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Generalized Least-Squares Evaluation of Nuclear Data Covariance Matrices of the Uncertainties of Experimental and Evaluated Data

PRONYAEV V.G.
PPE
Obninsk
Russia

Generalized Least-Squares Evaluation of Nuclear Data

Vladimir G. PRONYAEV
Institute of Physics and Power Engineering
Obninsk, Russia

Lecture 1. Non-model evaluation of experimental data: GLUCS and GMA codes

Lecture 2. Covariance matrices of uncertainties of experimental and evaluated data

CONTENT OF THE LECTURE 1

- Error (uncertainty) propagation law
- Generalized and Bayesian least-squares fit of the nuclear data
- Construction of the covariance matrices of the uncertainties of the experimental data
- Requirements to the covariance matrices of the uncertainties of the experimental and evaluated data
- Use of Bayesian code GLUCS for combined fit of the cross sections
- Bayesian approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions
- GMA code and simultaneous (combined) evaluation of neutron cross section standards, actinides cross sections and prompt fission neutron spectra

CONTENT OF THE LECTURE 2

- Covariance matrix of uncertainties obtained in non-model and model fits of the same experimental data and Peelle's effect
- Peelle's (PPP) effect and minimization of its influence at the bias of the evaluation
- Effect of small uncertainties of the evaluated data. Reasons leading to the small uncertainties
- Comparison of the covariance matrices of the uncertainties evaluated in the model and non-model fits and search of invariants of the uncertainties

- Questions and discussions

Own experience with the nuclear data (mostly neutron cross section) evaluation

1972 – 1980 Statistical and direct reaction theories/models and programming for calculation and evaluation of the cross sections (OM, Hauser-Feshbach with widths fluctuation and correlation , second order DWBA for reactions and RPA with phenomenological pairing for 1-phonon excitations in spherical nuclei (for structure), contribution of one and multi-phonon excitations in the neutron and proton scattering – semi-microscopic version of the Tamura-Udagawa-Lenske approach to multi-step direct pre-equilibrium). Contribution in the evaluation of BROND-1 library (structural materials) based on model calculations and own codes
1980-1984 Use of nuclear structure approach to nuclear reactions. Selection and compilation of the INDL (IAEA) – pre-ancestor of the FENDL

Own experience with the nuclear data (mostly neutron cross section) evaluation

1984 – 1992 Development of the multi-channel coupling model and semi-microscopic calculations of cross sections with ECIS with inclusion of the multi-phonon spaces. Evaluation of major structural materials for BROND-2 and materials important for (INTOR) ITER project.

1992 – 1997 Co-operation IRK (Vienna)/IPPE (Obninsk) for JEFF project. Work with GLUCS code for combined evaluation of integral cross sections and TNG code secondary energy angular distributions. Evaluation and preparation of the files for structural materials with covariance matrices of the uncertainties for cross sections, angular and energy distributions

2002 – 2006 International Neutron Cross Section Standard project (scientific secretary and work with the data and GMA)

Own experience with the nuclear data (mostly neutron cross section) evaluation

2005 – present Cooperation with the BNL/NNDC on fission products evaluations (mainly checking), ROSFOND project, further development of the standard project (including ^{252}Cf(sf) prompt fission neutron spectrum standard and ^{235}U(n_{th},f) PFNS as recommended spectrum, evaluation of major cross sections for minor actinides (including covariance matrices of the uncertainties)

Although I have practical experience in the least-squares fit of the nuclear data, I never worked in the mathematical statistics (as some my co-workers on standard project: Nancy Larson, Evgeny Gai)

Lecture 1

Uncertainty Propagation Law

If:

r_i - primarily-measured quantity in the point i
$d_i = D(r_i)$ – data reduced using reduction function $D(r_i)$
$\delta d_i = (\partial D_i / \partial r_k)\, \delta r_k$ – variation of reduced data (with summation on k)
$\partial D_i / \partial r_k$ – partial derivative

Then the averaged value of the product of the variations (variance-covariance):
$\langle \delta d_i \delta d_j \rangle = \langle (\partial D_i / \partial r_k)\, \delta r_k \delta r_l (\partial D_j / \partial r_l) \rangle$ (with summation on k and l)
can be written as:
$\langle \delta d_i \delta d_j \rangle = (\partial D_i / \partial r_k) \langle \delta r_k \delta r_l \rangle (\partial D_j / \partial r_l)$

Uncertainty Propagation Law

With designations of variances-covariances as $d_{ij}=<\delta d_i \delta d_j>$ and $r_{kl}=<\delta r_k \delta r_l>$:

$$d_{ij} = \sum_k \sum_l \frac{\partial D_i}{\partial r_k} r_{kl} \frac{\partial D_j}{\partial r_l} = D_{ik} r_{kl} D_{lj}$$

is an **uncertainty propagation law**, which connects **derived** quantity (e.g. cross section) wit the **primarily** measured quantities (e.g. number of counts); the similar equation is true for uncertainty propagation in the case of the model fit, where r_i are parameters, d_k are the values of the evaluated functions ($i<k$) and $\partial D_i/\partial r_k$ are sensitive coefficients

Generalized and Bayesian approaches to the least-squares fit of the nuclear data

- Both used in the model or non-model fits
- Model fit – mathematical or physical parametric model, matrix of sensitivity coefficients connects parameters with data values
- Non-model fit – data values reduced to the same nodes in the energy and are the parameters themselves, matrix of the sensitivity coefficients is the unit matrix
- Bayesian approach uses the conception of “prior” and “posterior” evaluations and sequential improvement of the posterior evaluations with account of next experimental data set
- Generalized fit does not need a prior evaluation, although on technical reasons an uninformative prior used to avoid “empty” values in the nodes

Generalized and Bayesian approaches to the least-squares fit of the nuclear data

- Examples of the implementation of these approaches at the level of the programming in the Standards project:
- R- matrix model codes using generalized least-squares method: EDA, RAC
- R- matrix model codes using Bayesian least-squares method: SAMMY
- Non-model codes using generalized least-square method: GMA, SOK
- Non-model code using Bayesian least-squares method : GLUCS

Generalized and Bayesian approaches to the least-squares fit of the nuclear data

Generalized approach [1]

$T' = (G^{+} V^{-1} G)^{-1} G^{+} V^{-1} R$

$M' = (G^{+} V^{-1} G)^{-1}$

Bayesian approach[2]

$T' = T + \delta T = T + MG^{+}(GMG^{+} + V)^{-1}(R - T)$

$M' = M + \delta M = M - MG^{+}(GMG^{+} + V)^{-1} GM$

where

T' is a vector of ("posteriori") evaluated data,

T is a vector of "priori" evaluated data,

M' is a covariance matrix of uncertainties of (posteriori) evaluated data,

M is a covariance matrix of uncertainties of (priori) evaluated data,

R is a vector of experimental data,

V is a covariance matrix of uncertainty of the experimental data,

G is a matrix of the coefficients of the data reduction or the model, upper indexes (+) and (-1) means the operators of the matrix transposing or inversion

Generalized and Bayesian approaches to the least-squares fit of the nuclear data

Scheme of Bayesian fit:

«a priori» evaluation (1) + experimental data (1) —> «a posteriori» evaluation (1)
«a priori» evaluation (2) (=evaluation (1)) + experimental data (2) —> «a posteriori» evaluation (2)

«priori» evaluation (n) (=evaluation (n-1)) + experimental data (n) —> final evaluation

Important peculiarities of Bayesian fit:

- Result of the fit does not depend from the order in which the experimental data are introduced
- No correlations between sequentially introduced experimental data
- Generalized and Bayesian approaches lead strictly to the same evaluation in the non-model fit, if used prior is non-informative or is an experimental data set presented in all energy nodes (**proof by N. Larson**)

Construction of covariance matrices of the uncertainties of the experimental data

- Most consistent approach - use of **uncertainty propagation law** to the equation of reduction of **primarily measured quantities**. To large extent, the approach is implemented in the SAMMY R- matrix code.
- For most published and compiled (in EXFOR) experimental data the primarily measured quantities, their uncertainties and often the data reduction formulas are not available.
- What is often given:

Short Energy Range Correlation (SERC) components of the uncertainties, e.g., statistical

Large Energy Range Correlation (LERC) components of the uncertainties, e.g., in the sample mass, quantum yields

Medium Energy Range Correlation (MERC) components of the uncertainties, e.g., in the detector efficiency, some corrections

Construction of covariance matrices of the uncertainties of the experimental data

If $d_i=D(r_i,q_1,q_2,q_3,\ldots,q_m,p^i_1,p^i_2,p^i_3,\ldots,p^i_n)$ is data reduction equation, where d_i is a final data, and r_i is a primarily-measured quantity at the point i, and q_k and p^i_l are the parameters (k and l are indexes of the components of the uncertainty) having different correlative properties.
Then the elements of the covariance matrix V_{ij} can be written as:

$$V_{ij} = \langle \delta d_i \delta d_j \rangle = \delta_{ij} \frac{\partial D_i}{\partial r_i} \Delta^2 r_i \frac{\partial D_i}{\partial r_i} + \sum_k \sum_l \frac{\partial D_i}{\partial q_k} \langle \delta q_k \delta q_l \rangle \frac{\partial D_j}{\partial q_l} + \sum_k \sum_l \frac{\partial D_i}{\partial p^i_k} \langle \delta p^i_k \delta p^j_l \rangle \frac{\partial D_j}{\partial p^j_l}$$

where $\Delta^2 r_i$ is a mean-square of the variation of the primarily-measured quantity, δ_{ij} – Kronecker's delta-symbol, $\langle \delta q_k \delta q_l \rangle$ and $\langle \delta p^i_k \delta p^j_l \rangle$ - covariance matrices of parameters with different correlative properties and $|\partial D_i/\partial r_i|$, $|\partial D_i/\partial q_k|$, $|\partial D_i/\partial p^i_k|$ - partial derivatives.

Construction of covariance matrices of the uncertainties of the experimental data

It can be written as:

$$V_{ij} = \delta_{ij} \frac{\partial D_i}{\partial r_i} \Delta^2 r_i \frac{\partial D_i}{\partial r_i} + \sum_k \frac{\partial D_i}{\partial q_k} \Delta^2 q_k \frac{\partial D_j}{\partial q_k} + \sum_l \frac{\partial D_i}{\partial p_l^i} \Delta p_l^i C_{ij}^l \Delta p_l^j \frac{\partial D_j}{\partial p_l^j}$$

where $\Delta^2 q_k$ is a mean-square of the variation of the parameter, $<\delta p^i{}_k \delta p^j{}_l> = \delta_{kl} \Delta p^i{}_l C^l{}_{ij} \Delta p^j{}_l$ with $C^l{}_{ij}$ correlation matrix of parameter p_l .
It can be written in the SERC, LERC and MERC components as:

$$V_{ij} = \delta_{ij} (\Delta_{SERC} D_i)^2 + \sum_k \Delta_{LERC} D_i^k \Delta_{LERC} D_j^k + \sum_l \Delta_{MERC} D_i^l C_{ij}^l \Delta_{MERC} D_j^l$$

Using absolute uncertainties Δ: $V_{ij} = \delta_{ij} \Delta_{Si}^2 + \sum_k \Delta_{Li}^k \Delta_{Lj}^k + \sum_l \Delta_{Mi}^l C_{ij}^l \Delta_{Mj}^l$

Construction of covariance matrices of the uncertainties of the experimental data

In presentation of absolute uncertainties and correlation matrices covariance matrix of the uncertainties of experimental data:

$$V_{ij} = \Delta^2_{Si} C_{Sij} + \sum_k \Delta^k_{Li} C_{Lij} \Delta^k_{Lj} + \sum_l \Delta^l_{Mi} C^l_{Mij} \Delta^l_{Mj}$$

Square correlation matrices C_{Sij} *(SERC)* and C_{Lij} (LERC) has a strict form, and C_{Mij} (MERC) depends from correlation length of components of the uncertainties and phenomenological way of assigning the point-to-point correlations

$$C_{Sij} = \begin{vmatrix} 1.0 & 0.0 & 0.0 \ldots\ldots 0.0 \\ 0.0 & 1.0 & 0.0 \ldots\ldots 0.0 \\ 0.0 & 0.0 & 1.0 \ldots\ldots 0.0 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ 0.0 & 0.0 & 0.0 \ldots\ldots 1.0 \end{vmatrix} \quad C_{Lij} = \begin{vmatrix} 1.0 & 1.0 & 1.0 \ldots\ldots 1.0 \\ 1.0 & 1.0 & 1.0 \ldots\ldots 1.0 \\ 1.0 & 1.0 & 1.0 \ldots\ldots 1.0 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ 1.0 & 1.0 & 1.0 \ldots\ldots 1.0 \end{vmatrix} \quad C_{Mij} = \begin{vmatrix} 1.0 & 0.9 & 0.7 \ldots\ldots 01 \\ 0.9 & 1.0 & 0.8 \ldots\ldots 02 \\ 0.7 & 0.8 & 1.0 \ldots\ldots 03 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ 0.1 & 0.2 & 0.3 \ldots\ldots 10 \end{vmatrix}$$

Construction of covariance matrices of the uncertainties of the experimental data

- Correlation function for each MERC component of the uncertainty is modelled usually with linear type function, which describes the correlation of the uncertainties between two energy points. The length of correlations for each component is chosen as some minimal distance between two energy points, where correlation between uncertainties is negligible.
- Total covariance matrix of the uncertainties of experimental data obtained as sum of all components should be positive definite (have all eigenvalues positive) and be realistic as much as possible to avoid Peelle's Pertinent Puzzle (PPP) effect. This in details will be discussed later. Because of the symmetry of the square matrix, it is often only low triangle of the matrix is presented.

Construction of covariance matrices of the uncertainties of the experimental data

- The same methods, detectors or samples can be used in different measurements done by the same group of the experimentalists. This leads to noticeable correlations between the uncertainties in these measurements. Then correlations between data sets are introduced.
- The correlated data sets should be combined in the data blocks with introducing of the coefficients of correlation between components of the uncertainties of different data sets
- Practical example: standards data for two sets of absolute ratio measurements $^{235}U(n,f)/^{238}U(n,f)$ prepared by Wolfgang Poenitz for GMA database: 100% correlations in the uncertainty of the sample masses, 80% correlations in the uncertainty of the efficiency of the detector and 50% correlations in the uncertainty of the corrections at scattering and the absorption

Construction of covariance matrices of the uncertainties of the experimental data

```
DATABLOCK**************************
DATASET***************************
  DATA SET  853  RATIO              U8(n,f)           U5(n,f)
  YEAR 1983 TAG  1 AUTHOR:  A.A.GOVERDOVSKII ET AL.              83KIEV,159 (1984)
  ENERGY/MEV   VALUE    ABS. UNCERT.   PRIOR/EXP UNCERT./%    DIFF./%  VAL.*SQRT(E)
  0.5500E+01  0.5020E+00  0.2385E-01   1.0496      4.8          -4.7       1.1773
  0.5800E+01  0.5423E+00  0.1065E-01   1.0099      2.0          -1.0       1.3060
  0.6200E+01  0.5807E+00  0.1112E-01   0.9977      1.9           0.2       1.4459
  0.6500E+01  0.6068E+00  0.1070E-01   1.0104      1.8          -1.0       1.5470
  0.7000E+01  0.6037E+00  0.1083E-01   1.0104      1.8          -1.0       1.5972
  0.7500E+01  0.5743E+00  0.9780E-02   1.0119      1.7          -1.2       1.5728
  0.7750E+01  0.5715E+00  0.1095E-01   0.9970      1.9           0.3       1.5910
  0.8000E+01  0.5674E+00  0.1062E-01   0.9989      1.9           0.1       1.6048
  0.8500E+01  0.5612E+00  0.9897E-02   1.0031      1.8          -0.3       1.6362
  0.9000E+01  0.5631E+00  0.9786E-02   1.0092      1.7          -0.9       1.6893
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  DATA SET  854  RATIO              U8(n,f)           U5(n,f)
  YEAR 1984 TAG  1 AUTHOR:  A.A.GOVERDOVSKII ET AL.              AE 56,164(1984)
  ENERGY/MEV   VALUE    ABS. UNCERT.   PRIOR/EXP UNCERT./%    DIFF./%  VAL.*SQRT(E)
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  0.1450E+02  0.5568E+00  0.1610E-01   1.0204      2.9          -2.0       2.1202
  0.1500E+02  0.5499E+00  0.2197E-01   1.0597      4.0          -5.6       2.1298
DATABLOCK*************************************************************
```

Construction of covariance matrices of the uncertainties of the experimental data

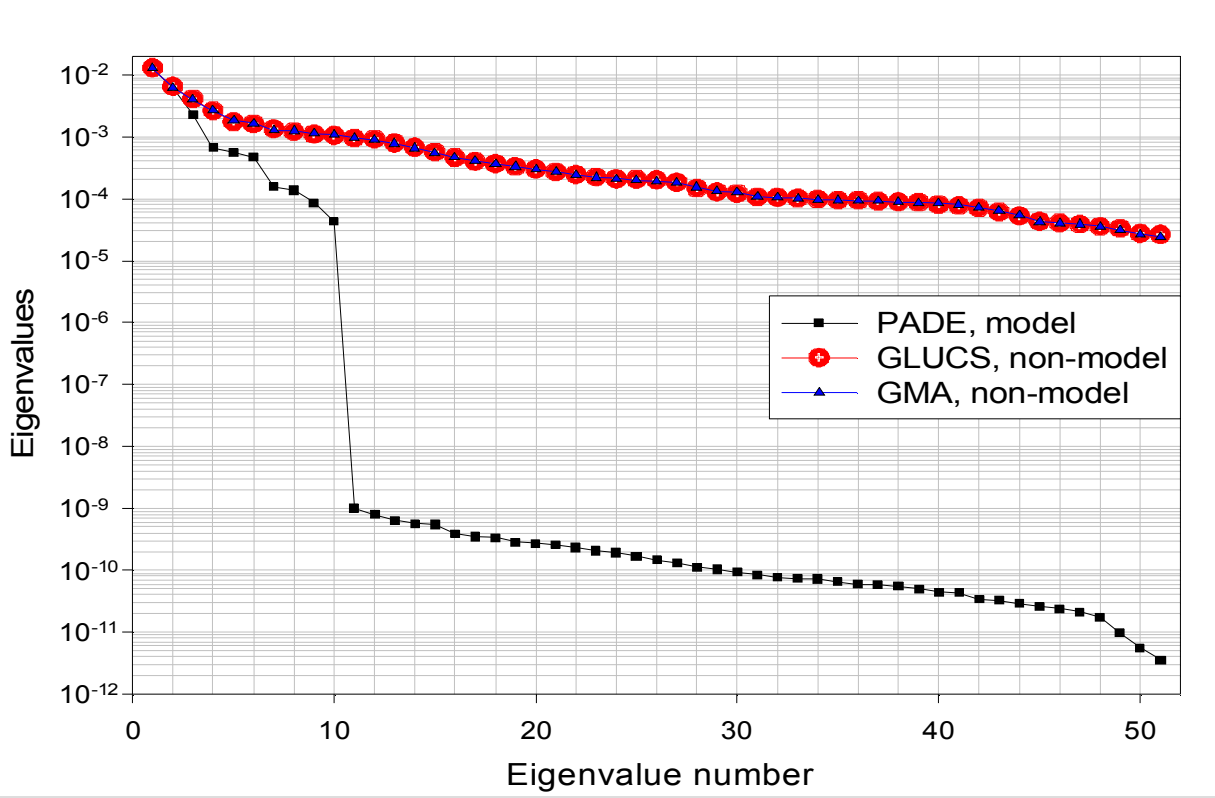
```
 CORRELATION MATRIX OF DATA BLOCK
1.00
0.29 1.00
0.27 0.70 1.00
0.28 0.73 0.80 1.00
0.25 0.65 0.72 0.83 1.00
0.25 0.64 0.71 0.81 0.87 1.00
0.23 0.55 0.60 0.69 0.74 0.84 1.00
0.23 0.56 0.60 0.68 0.73 0.83 0.77 1.00
0.25 0.59 0.61 0.68 0.72 0.83 0.76 0.81 1.00
0.25 0.60 0.62 0.67 0.69 0.79 0.72 0.77 0.87 1.00
0.25 0.60 0.62 0.67 0.66 0.69 0.64 0.68 0.78 0.84 1.00
0.11 0.27 0.28 0.30 0.29 0.31 0.28 0.29 0.30 0.30 0.30 1.00
0.09 0.23 0.24 0.26 0.25 0.27 0.24 0.25 0.26 0.26 0.26 0.77 1.00
0.07 0.17 0.17 0.19 0.18 0.19 0.17 0.18 0.19 0.19 0.19 0.52 0.85 1.00

 DATABLOCK**************************************************************
```

Inclusion of cross-reaction correlations leads to large increase of the dimensions of the covariance matrix of the evaluated data

Requirements to the covariance matrices of the uncertainties of the experimental and evaluated data

- Only positive (all eigenvalues are positive) and semi-positive (eigenvalues are positive or zeros) definite covariance matrix of the uncertainties of experimental data guarantees the positive uncertainties of quantities calculated with these data.
- This should be accounted by such a way that all numerical schemes of matrix calculations should not lead to the loss of accuracy.
- This is especially important for large covariance matrices with large difference in the maximal (λ_{max}) and minimal (λ_{min}) values of the eigenvalues.
- Calculations at single precision at 32-bits machine for matrices with $\lambda_{max}/\lambda_{min}$ more than 6 decimal order of magnitude and rounding of the covariance (correlation matrices) may create the problems.

Requirements to the covariance matrices of the uncertainties of the experimental and evaluated data



ACORNS code for calculation of egenvalues at 32-bit PC:

51 data points

51 eigenvalues for non-model fit (positive definite)

10 eigenvalues for model fit (semi-positive definite)

Eigenvalues with numbers 11-51 are machine zeros (are given as computer garbage)

Eigenvalues of the covariance matrices of the uncertainty of the ^{6}Li(n,t) cross section evaluated in the model (PADE, 10 parameters) and non-model (GMA, GLUCS) least-squares fits.

Requirements to the covariance matrices of the uncertainties of the experimental and evaluated data

The size of present matrices in the combined evaluation of the standards with GMA code is 1200*1200.

For calculations (including the matrix inversion) double precision at 64-bits machines were used (DECAlpha with OpenVMS).

Code was recompiled with COMPAQ Fortran compiler with double precision at 32-bits PC (64-bits co-processor). No difference above 6 digits were found in the fit of the large standard data base.

The natural strict requirements for covariance matrices of the uncertainties is inequality $V_{ij} \leq \sqrt{V_{ii} V_{jj}}$

Another requirement for the PPP exclusion will be discussed later

Use of Bayesian code GLUCS for combined fit of the cross sections and covariances for neutron-induced reactions

• **GLUCS** – the Bayesian program complex developed at ORNL (USA) and updated by S. Tagesen (IRK, Austria) for combined evaluation of all cross sections for one nuclei.

• Includes 3 codes:

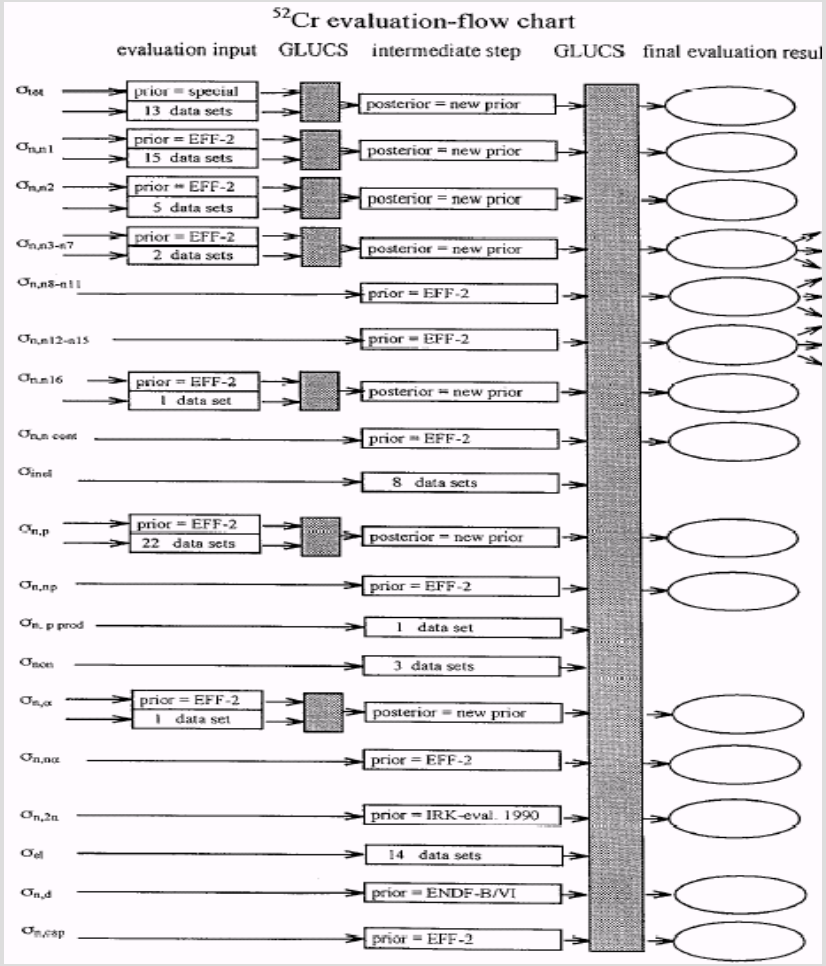
INPUT – reads a prior cross sections and covariances from ENDF-6 formatted files

GLUCS – fits using least-squares approach the experimental data sets prepared by some auxiliary programs

OUTPUT – convert the GLUCS output in the ENDF-6 formatted posterior evaluation

• Constraints and physical relations between partial and total cross sections are accounted

Use of Bayesian code GLUCS for combined fit of the cross sections and covariances for neutron-induced reactions



Example of ^{52}Cr+n evaluation with Bayesian inclusion of new data:

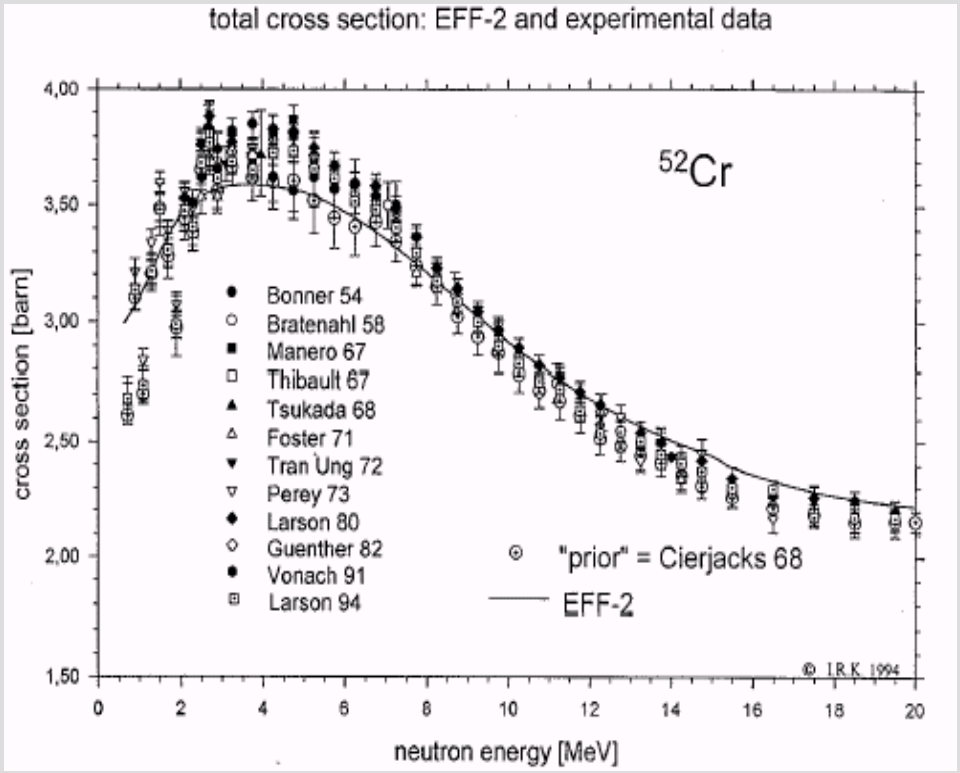
The neutron energy interval for **all r eactions** included is between **0.64 and 20 MeV**.

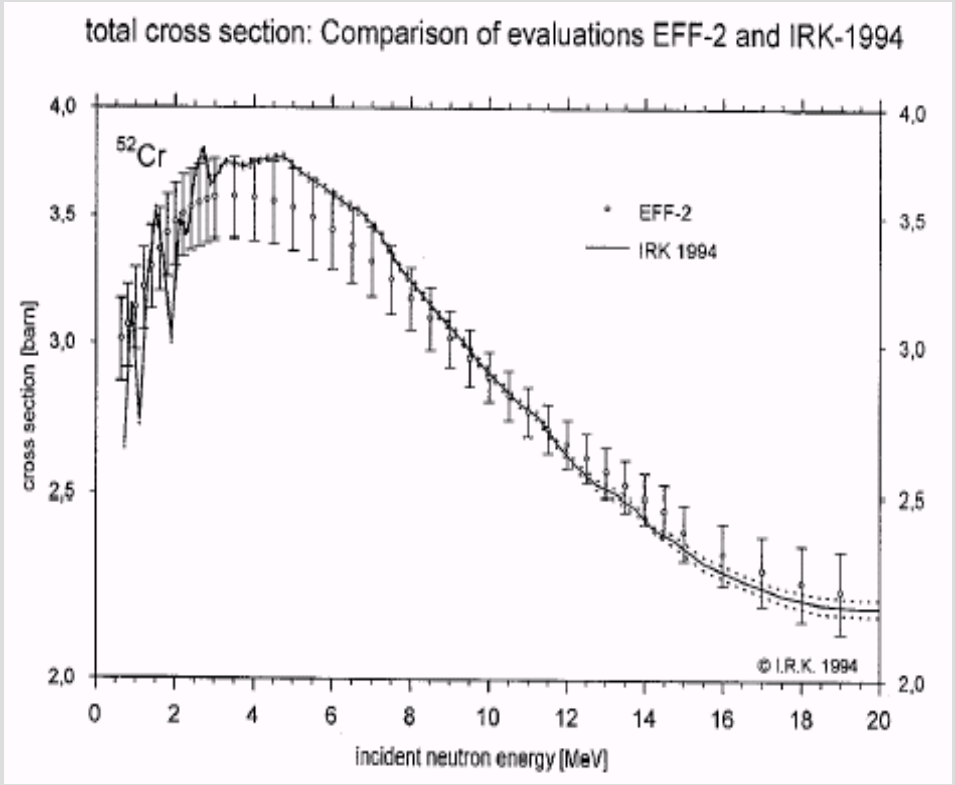
Some old evaluation (mostly from EFF-2) was taken as a prior for all reaction channels with a rather large (non-informative) prior uncertainties.

At the **first ste p** the partial channels for which the experimental data are available have been evaluated.

At the **second step**, all other reactions and constraints/relations between partial and total cross sections have been added in the fit (total inelastic scattering, non-elastic and total cross section).

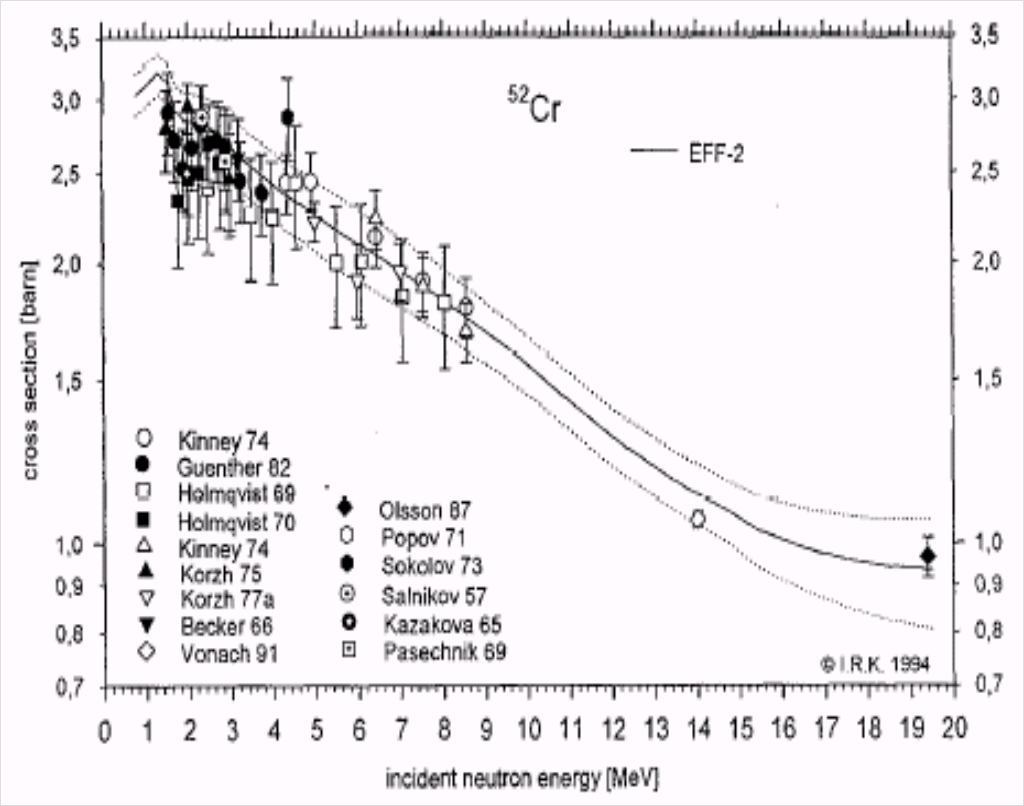
Use of Bayesian code GLUCS for combined fit of the cross sections and covariances for neutron-induced reactions

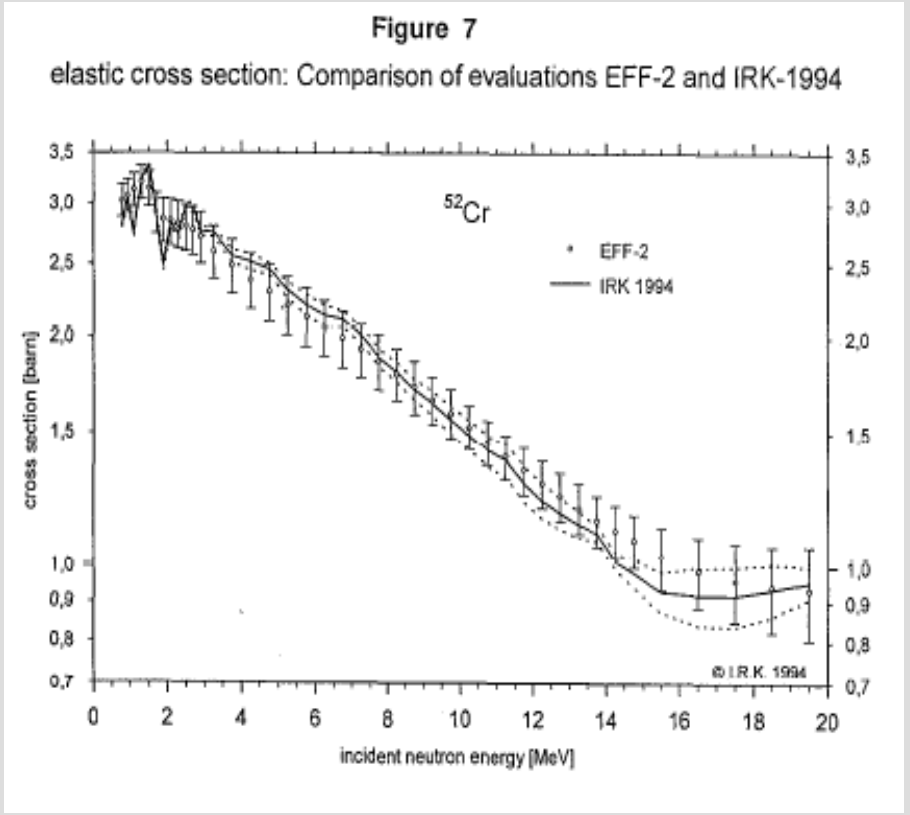




Evaluation of ^{52}Cr+n total cross section

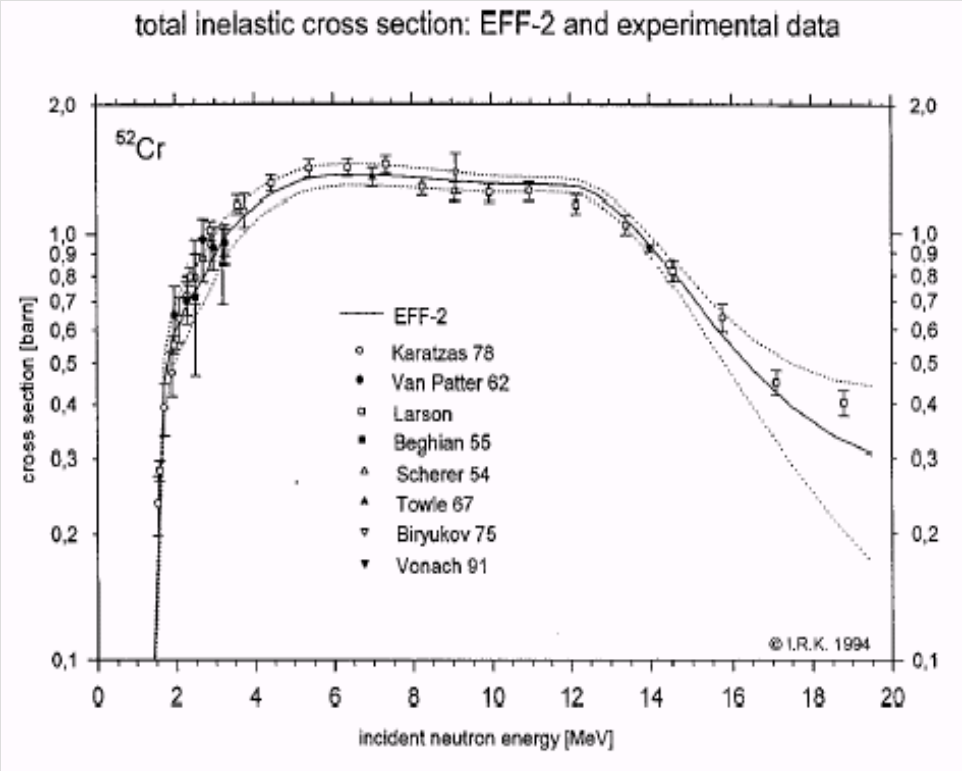
Use of Bayesian code GLUCS for combined fit of the cross sections and covariances for neutron-induced reactions

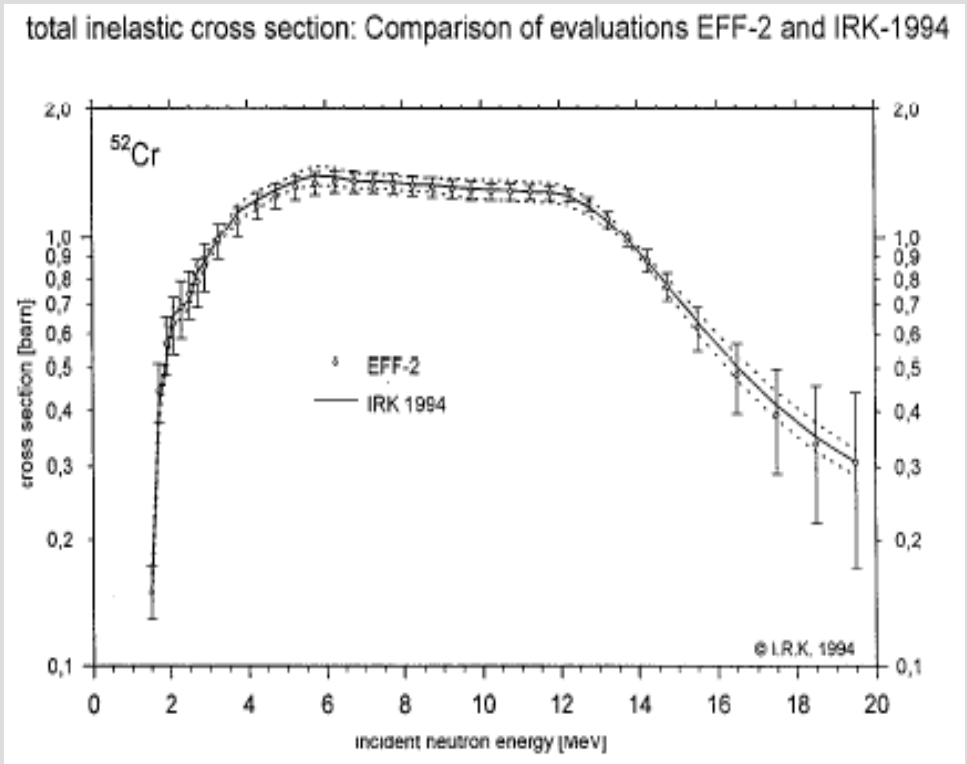




Evaluation of ^{52}Cr+n elastic scattering cross section

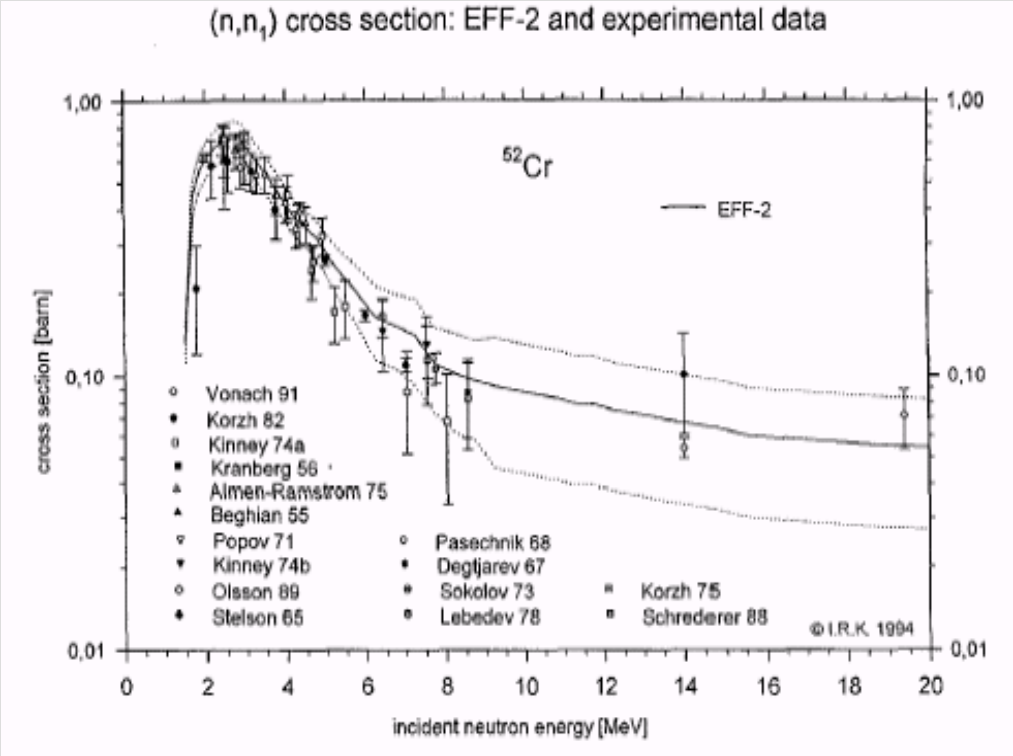
Use of Bayesian code GLUCS for combined fit of the cross sections and covariances for neutron-induced reactions

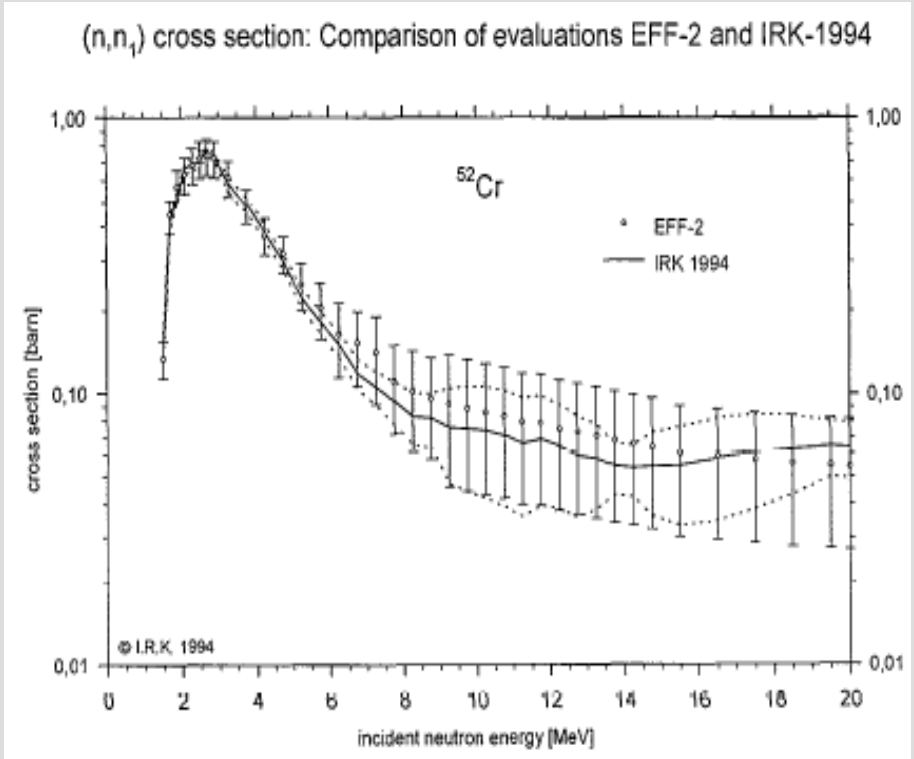




Evaluation of ^{52}Cr+n total inelastic scattering cross section

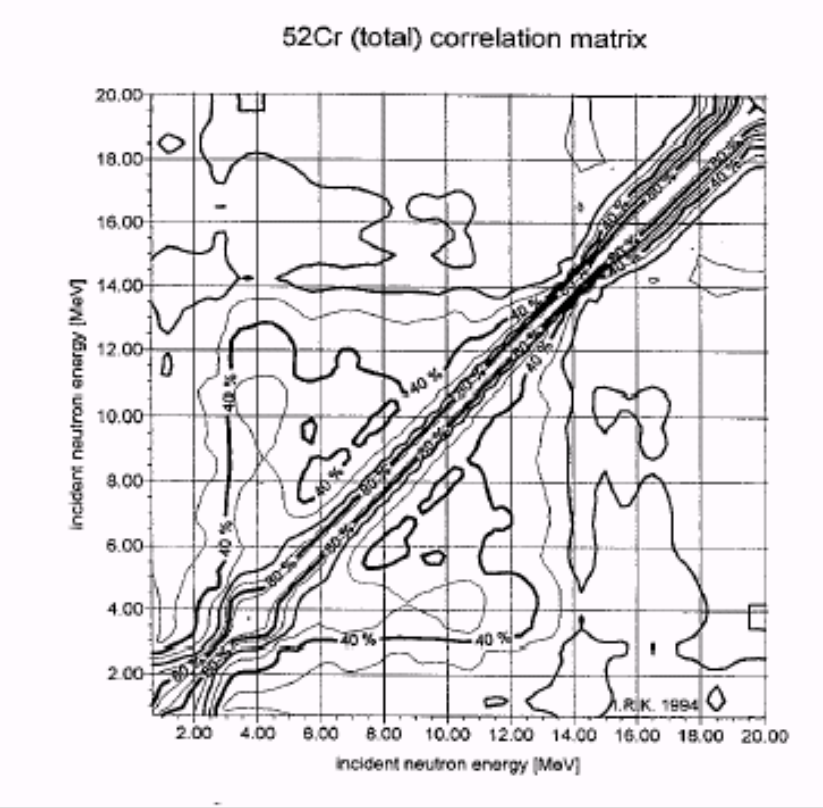
Use of Bayesian code GLUCS for combined fit of the cross sections and covariances for neutron-induced reactions

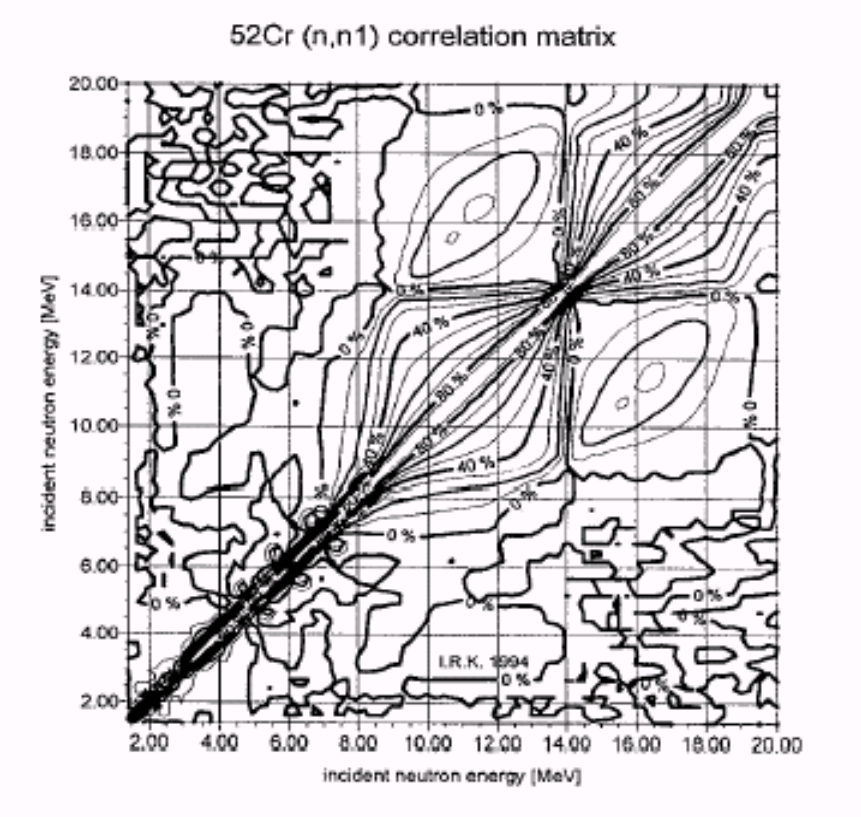




Evaluation of ^{52}Cr+n inelastic scattering cross section with excitation of the first level

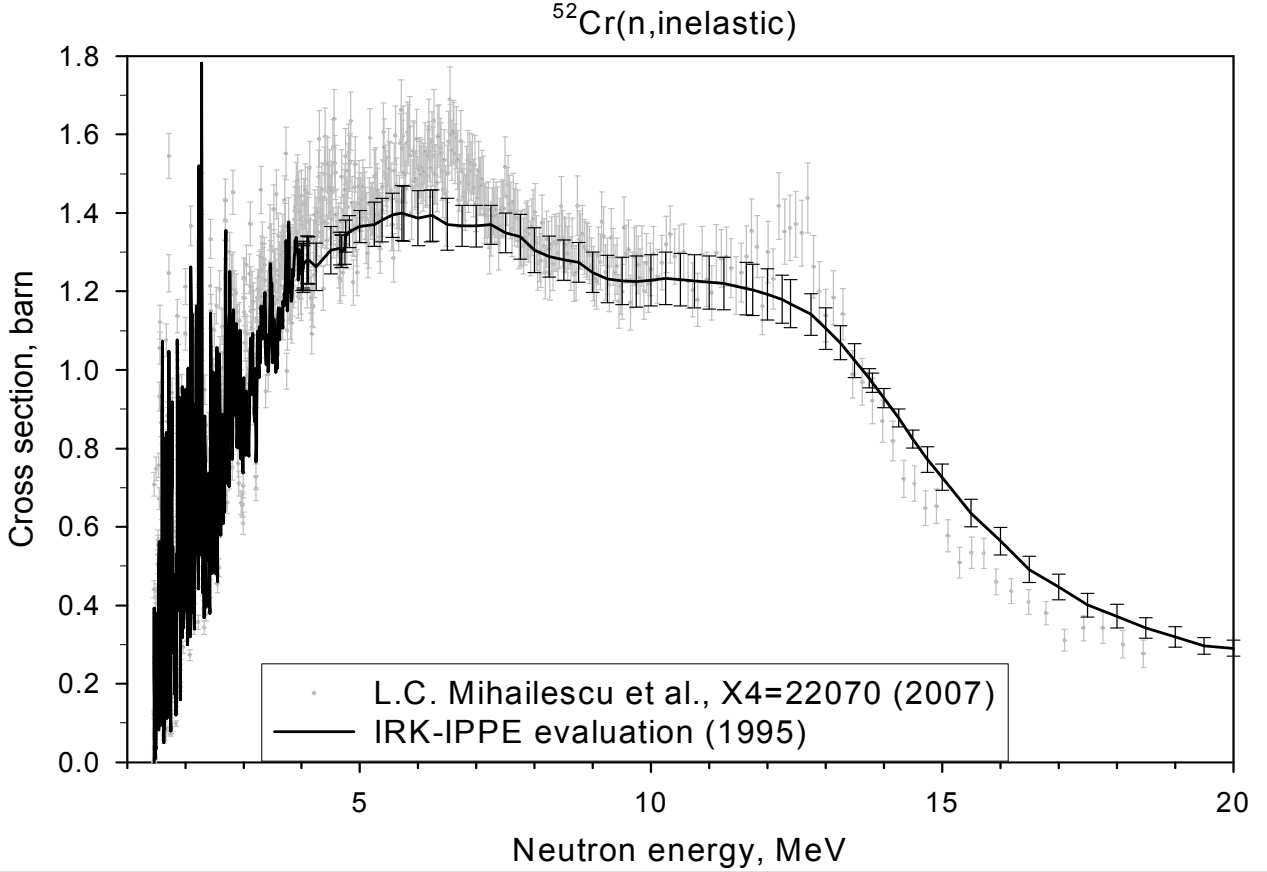
Use of Bayesian code GLUCS for combined fit of the cross sections and covariances for neutron-induced reactions





Correlation matrices of the evaluated uncertainties for total and inelastic scattering cross section with the excitation of the first level.

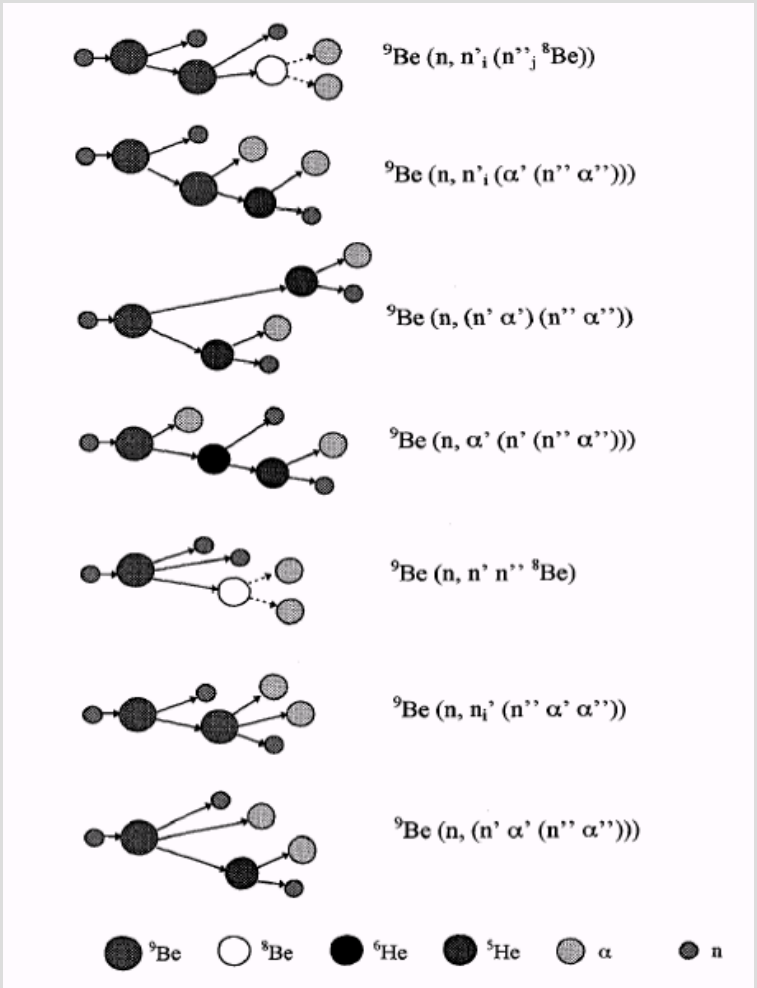
Use of Bayesian code GLUCS for combined fit of the cross sections and covariances for neutron-induced reactions



Comparison of the 1434.07 keV gamma-line production cross section (γ-transition between first excited and ground state is about 95% of total inelastic scattering at ^{52}Cr).

"Bench-marking" of 1995 evaluation with the results of the modern experiment.

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions

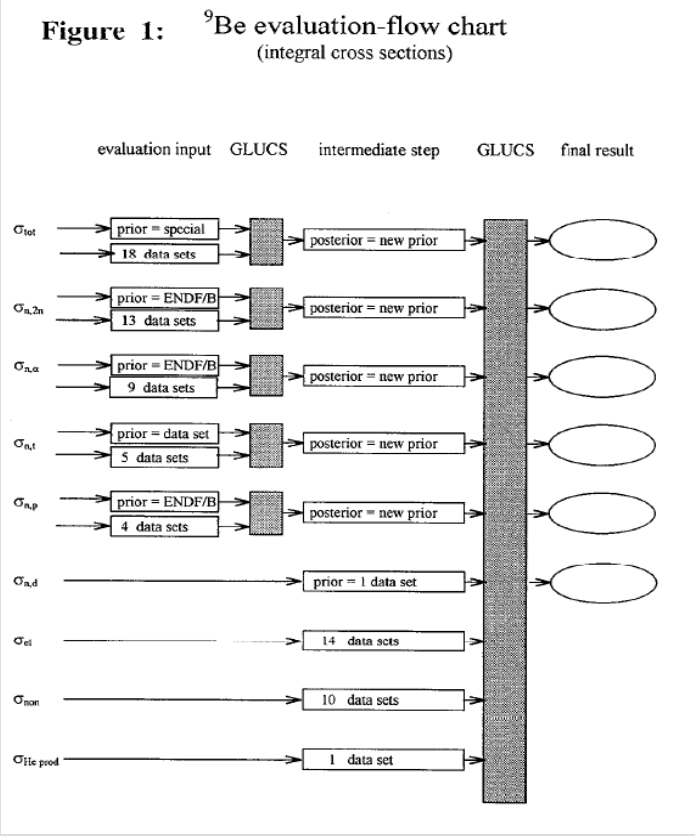


Main mechanisms of the reactions of interaction of neutrons with energy above 2 MeV with ^{9}Be lead to break-up of the ^{10}Be compound system at 2 neutrons and 2 alpha-particles.

^{8}Be residual nuclei decays for nuclear time at two alpha-particles ($\Gamma(\alpha-\alpha)=6.7$ eV).

^{9}Be is a good neutron multiplier for thermonuclear hybrid installations; the evaluation should be done for cross sections in all channels and secondary energy angular distributions.

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions



N	Elev, MeV	Jp	Γ_{tot}, MeV	Branching Ratio for decay to final state				
				^{8}Be g.s. BR1	^{8}Be 1-st BR2	^{5}He g.s. BR3	^{5}He 1-st BR4	(nαα)-3-body BR5
0	0.0 (g.s.)	3/2-	0.0(stable)	0.0	0.0	0.0	0.0	0.0
1	1.684	1/2+	0.217	1.00	0.0	0.0	0.0	0.0
2	2.4294	5/2-	0.00077	0.07	0.0	0.0	0.0	0.93
3	2.78	1/2-	1.08	1.00	0.0	0.0	0.0	0.0
4	3.049	5/2+	0.282	0.87	0.13	0.0	0.0	0.0
5	4.704	3/2+	0.743	0.13	0.87	0.0	0.0	0.0
6	5.59	3/2-	1.33	0.5	0.5	0.0	0.0	0.0
7	6.38	7/2-	1.21	0.02	0.55	0.43	0.0	0.0
8	6.76	9/2+	1.33	0.0	1.0	0.0	0.0	0.0
9	7.940	1/2-	1.00	0.5	0.5	0.0	0.0	0.0
10	11.283	9/2-	1.10	0.02	0.14	0.84	0.0	0.0
11	11.81	5/2+	0.400	0.20	0.80	0.0	0.0	0.0
12	13.79	5/2-	0.590	0.0	1.0	0.0	0.0	0.0
13	14.392	3/2-	0.000381	0.049	0.386	0.565	0.0	0.0
14	14.4	1/2-	0.8	0.5	0.5	0.0	0.0	0.0
15	15.1	7/2-	0.35	0.0	1.0	0.0	0.0	0.0
16	15.9	5/2-	0.31	0.0	1.0	0.0	0.0	0.0
17	16.672	5/2+	0.041	0.0	0.0	1.0	0.0	0.0
18	16.975	1/2-	0.00049	0.07	0.0	0.0	0.0	0.93
19	17.298	5/2-	0.20	0.0	1.0	0.0	0.0	0.0
20	17.493	7/2+	0.047	0.0	0.0	1.0	0.0	0.0

Evaluation flow chart for step 1 (left) and characteristics of the reactions with excitation of ^{9}Be levels in the inelastic scattering of neutrons(right).

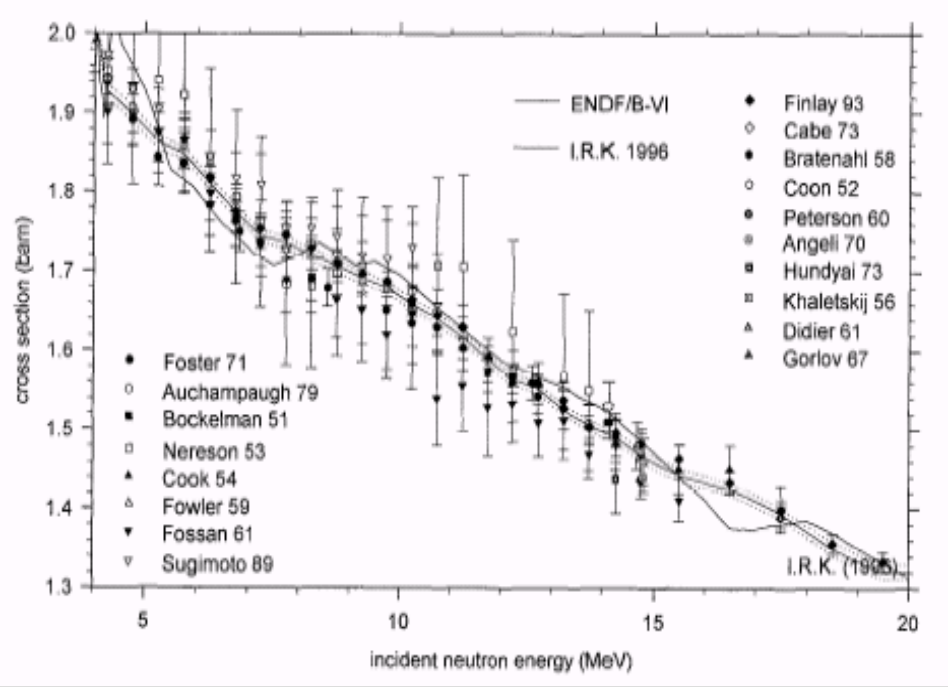
Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions

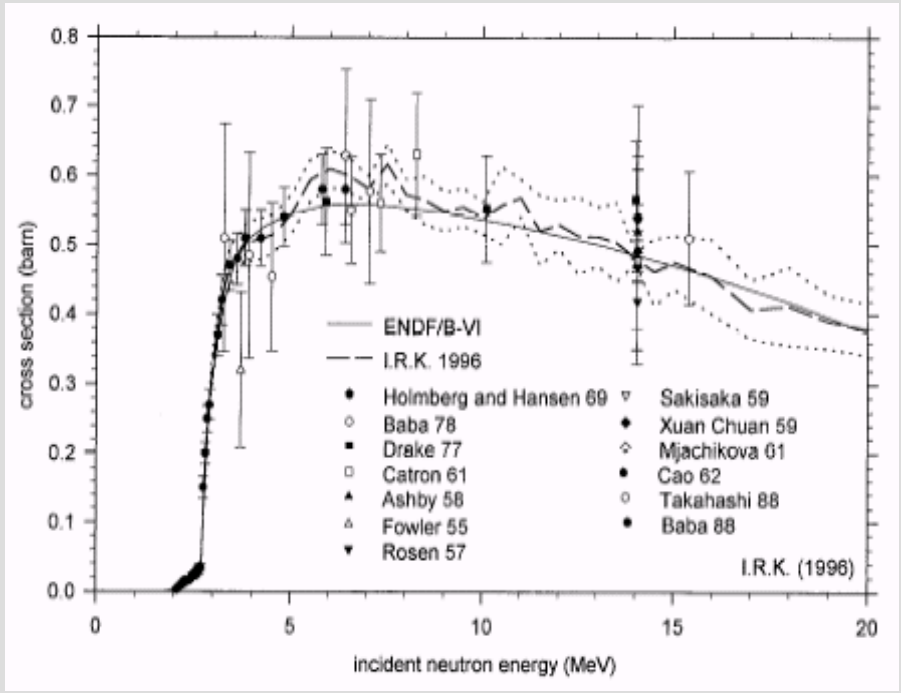
En	2.0	3.0	4.0	5.0	5.9	7.0	8.0	9.0	10.1	11.0	12.0	13.0	14.1	15.0	17.0	20.0
tot	2102	2003	1885	1842	1798	1754	1733	1722	1676	1640	1584	1528	1473	1436	1375	1315
ela	2010	1700	1389	1295	1218	1170	1135	1117	1094	1065	1037	1006	971	949	912	870
non	92	305	496	547	580	584	598	605	582	575	547	522	502	487	463	445
n,n1	31.3	46.9	38.0	36.0	31.5	24.1	19.8	15.5	11.6	9.90	8.17	6.98	5.43	4.63	3.45	2.06
n,n2		122	212	252	271	272	249	236	215	198	180	158	140	129	112	102
n,n3			23.6	22.6	21.5	19.2	18.8	15.8	12.0	10.3	8.53	7.23	5.43	4.60	3.73	2.60
n,n4			49.2	46.9	42.5	39.6	35.6	31.2	25.0	22.8	19.3	16.6	12.9	11.0	9.21	6.73
n,n5					16.4	16.9	17.4	16.7	14.7	14.4	12.9	11.6	9.19	7.94	6.47	4.69
n,n6						11.9	13.5	13.4	12.4	12.8	12.0	11.3	9.03	7.83	6.58	5.08
n,n7							50.1	65.2	72.1	79.7	82.1	79.0	77.6	75.1	70.5	64.7
n,n8							7.20	9.33	9.15	9.93	10.0	9.65	8.61	8.03	7.97	7.13
n,n9								1.49	3.68	3.67	3.59	3.59	3.31	3.14	2.88	2.46
n,n10												3.15	6.98	8.34	10.9	12.4
n,n11													4.50	4.69	4.55	5.05
n,n12															3.42	3.48
n,n13															1.89	2.31
n,n14															0.91	1.16
n,n15															0.80	3.62
n,n16																2.65
n,n17																2.27
n,n18																0.70
n,n19																1.59
n,n20																1.34
n,α0	45	105	85	65	50	35	28	22	19	17	15	13	11	10	8	5
n,α1		1.50	55.4	70.0	62.6	53.4	40.4	33.5	32.2	27.4	23.9	21.3	18.6	17.1	13.6	9.24
n,α2				4.2	25.1	36.4	32.1	31.1	34.0	30.8	28.3	26.6	24.5	23.3	19.5	14.4*
n,^{5}He^{5}He			5.0	22.0	31.0	37.0	36.0	33.0	28.0	24.0	19.0	14.0	10.0	8.0	5.0	5.0*
n,nn^{8}Be		16.0	22.0	25.0	27.0	29.0	31.0	33.0	34.0	36.0	37.0	38.0	39.0	40.0	41.0	42.0*
n,nα^{5}He					3.0	11.0	20.0	48.0	60.0	78.0	88.0	102	115	124	131	136*

Contribution of the 2-body (n,^{5}He^{5}He) and 3-body reactions (n,nn^{8}Be) and (n,na^{5}He) with no experimental data were obtained from consistency of total and partial cross sections by expert estimation and have large, non-informative covariance matrices of the uncertainties.

Posterior evaluation obtained after step 1 of integral cross section evaluation, added by ECIS and TNG codes calculations and experts estimations for 2- and 3-body break-up reactions.

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions





Comparison of the experimental and evaluated data for total and (n,2n) cross section obtained after the 1-step of evaluation of the integral cross sections.

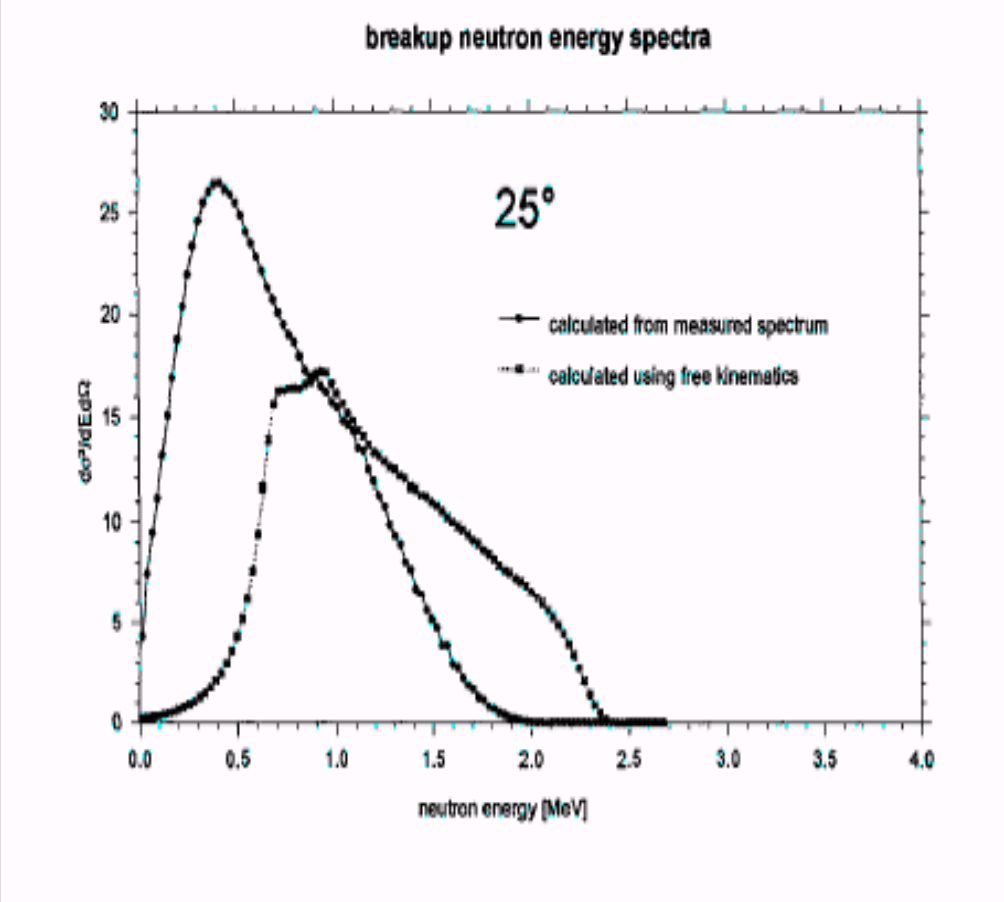
Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions

• At the next step of the evaluation we have used least-squares fit of the experimental data on neutron emission spectra at 4 initial energies (5.9, 10.1, 14.1 and 18.1 MeV) for a large number of angles.

• For multi-particle break-up calculations a free 2-body or 3-body break-up kinematics is used for obtaining of angular-energy distributions in the centre of mass system in cases if energy-angular distributions were not known from the experiment or model calculations.

• For transformation of the multi-step break-up processes from center of mass in the laboratory system the program using analytical formulas (where they were obtained) or using multiple numerical integration were used.

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions



Energy distribution for second neutron in ^{9}Be(n,n'(**n''**α'α")) reaction under the angle of 25 degree in the laboratory system in case of free-kinematics break up ^{9}Be* at two α-particles and neutron and with account of the interaction between particles as taken from the experiment.

More low and narrow spectrum is for free kinematic break up.

Coulomb interaction increases the energy of α-particles and reduces the energy of neutron.

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions

Adjustment of contribution of different channels in the least-squares fit of 5.9 MeV neurton emission spectrum using Bayesian procedure for each angle of neutron emission.

Channel	Prior c.s.	Posterior c.s.
(n,n'1)		
(n,α2)	25.1 (100.)	50.7 (49.)
(n,n'2)	271 (5.)	258 (4.6)
(n,n'(3+4)	58.8 (100.)	0
(n,n'5)	16.4 (100.)	18.4 (78.)
(n,α1)	62.6 (50.)	45 (40.)
(n,^{5}He^{5}He)	31 (100.)	44.6 (60.)
(n,n'n''^{8}Be)	27 (100.)	31.2 (80.)
(n,n'α^{5}He)	30 (100.)	57.8 (48.)

Correlation coefficients between uncertainties on different channels obtained in the fit

	1	2	3	4	5	6	7	8	9	10
1 (n,n1')	100									
2 (n,n2')	-12	100								
3 (n,n3')	0	5	100							
4 (n,n4')	-16	1	-51	100						
5 (n,n5')	3	-4	0	1	100					
6 (n,a1)	2	-24	0	0	-28	100				
7 (n,a2)	-12	0	0	-4	-7	-18	100			
8 (n,5He5He)	-4	1	0	-1	-12	-30	-20	100		
9 (n,n'n''8Be)	-25	-12	0	-9	-2	10	-14	-10	100	
10(n,n'a5He)	-11	0	0	-3	-12	-14	-22	-26	-24	100

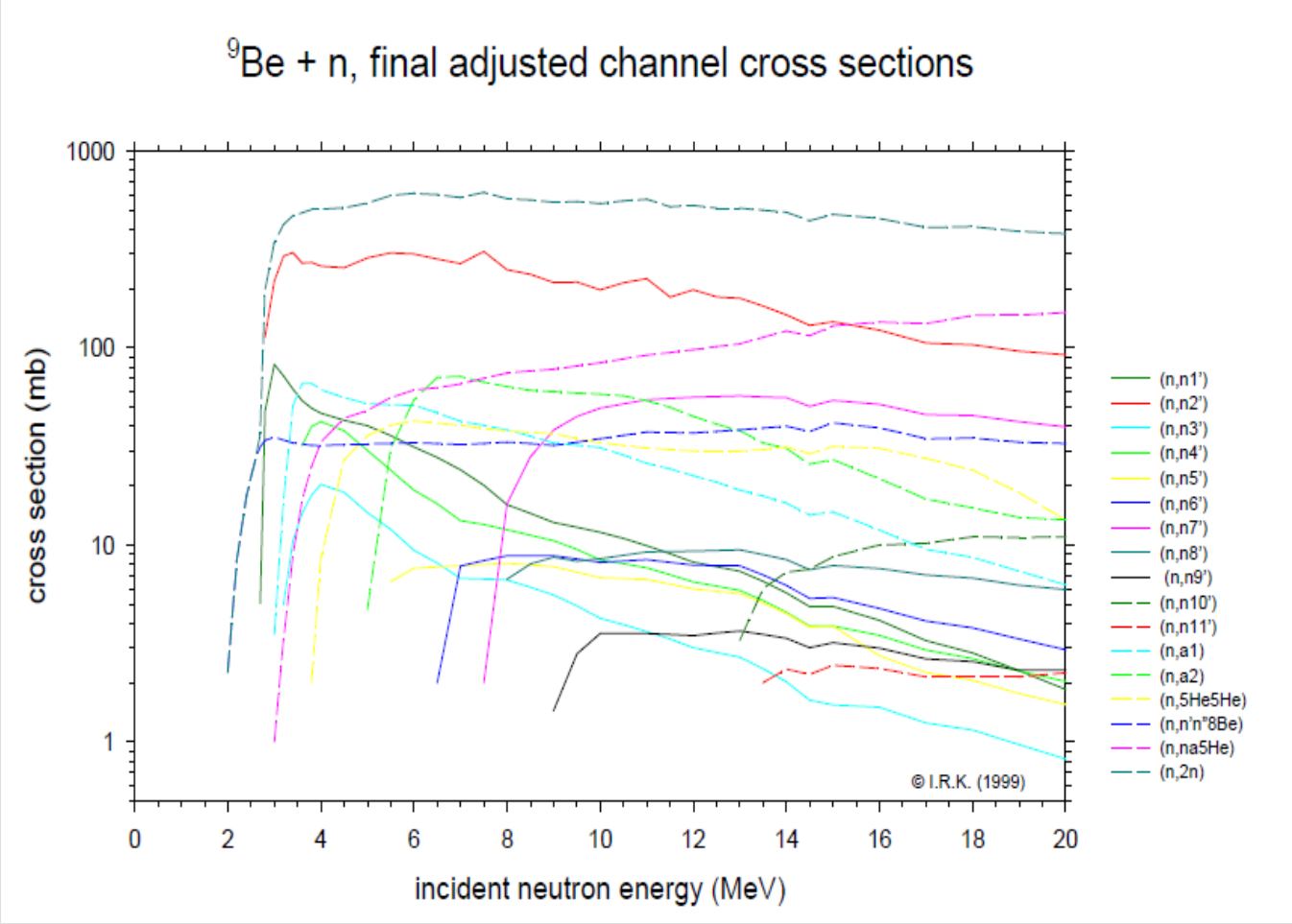
Correlations are negative (because of competition between contributions in the same range) or small (no competition)

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions

Correlation coefficients between uncertainties on different channels obtained in the fit of 18 MeV emission spectrum

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1 (n,n1‘)	100															
2 (n,n2‘)	-7	100														
3 (n,n3‘)	-1	2	100													
4 (n,n4‘)	-3	-11	0	100												
5 (n,n5‘)	-1	-6	0	-1	100											
6 (n,n6‘)	0	3	0	0	0	100										
7 (n,n7‘)	-3	-25	0	-5	-3	-32	100									
8 (n,n8‘)	2	7	-3	1	0	-32	-31	100								
9(n,n9‘)	0	-3	-5	0	0	-7	12	0	100							
10(n,n10‘)	0	-6	-5	-1	0	-7	10	0	0	100						
11(n,n11‘)	0	-2	-5	0	0	-7	13	0	0	-30	100					
12(n,a1)	-1	-1	-35	0	0	0	0	0	0	-2	0	100				
13(n,a2)	0	-4	8	0	0	-22	12	0	0	-33	0	15	100			
14(n,5He5He)	0	0	9	0	0	-5	0	0	0	-9	0	15	-34	100		
15(n,n’n''8Be)	0	-1	15	0	0	-6	2	0	0	-45	0	53	64	18	100	
16(n,n’a5He)	-3	-25	-11	-5	-3	12	-15	3	-2	34	-1	-53	-68	-13	-89	100

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions

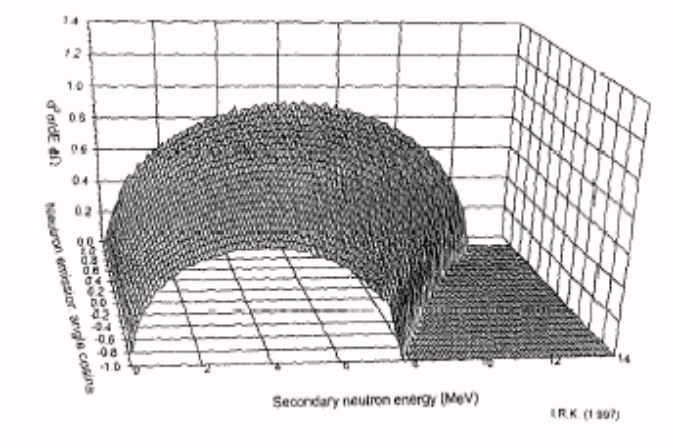


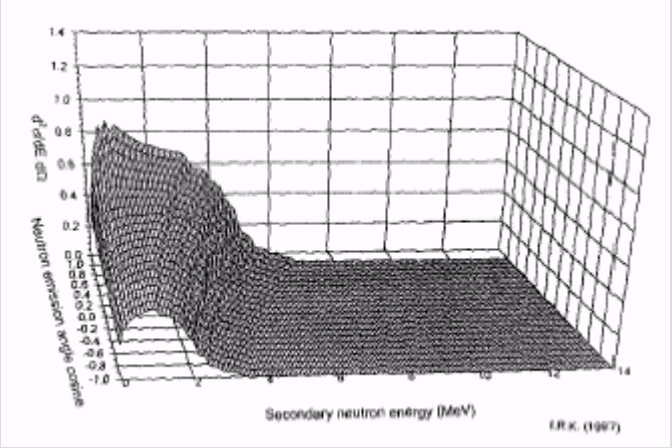
After adjustment of channel crossections using energy angular distributions at 5.9, 10.1, 14.1 and 18.1 MeV, the interpolation with smoothing of channels contribution was done.

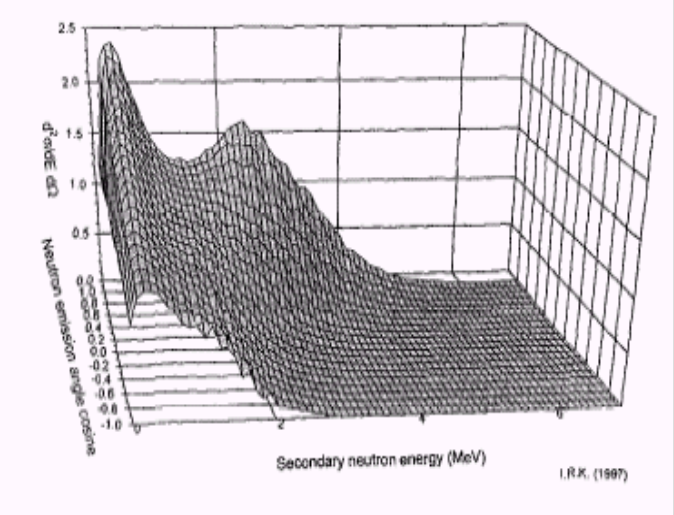
Using these values the calculations of spectra in 39 nodes on energy were done for evaluated data file.

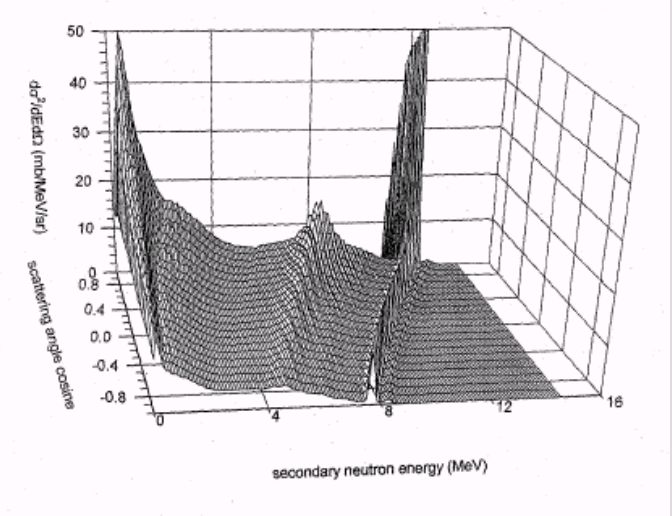
File included covariance matrices for cross sections and energy-angular distributions.

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions









Results of the evaluation of the energy-angular distributions in laboratory system at 14 MeV incident neutrons :

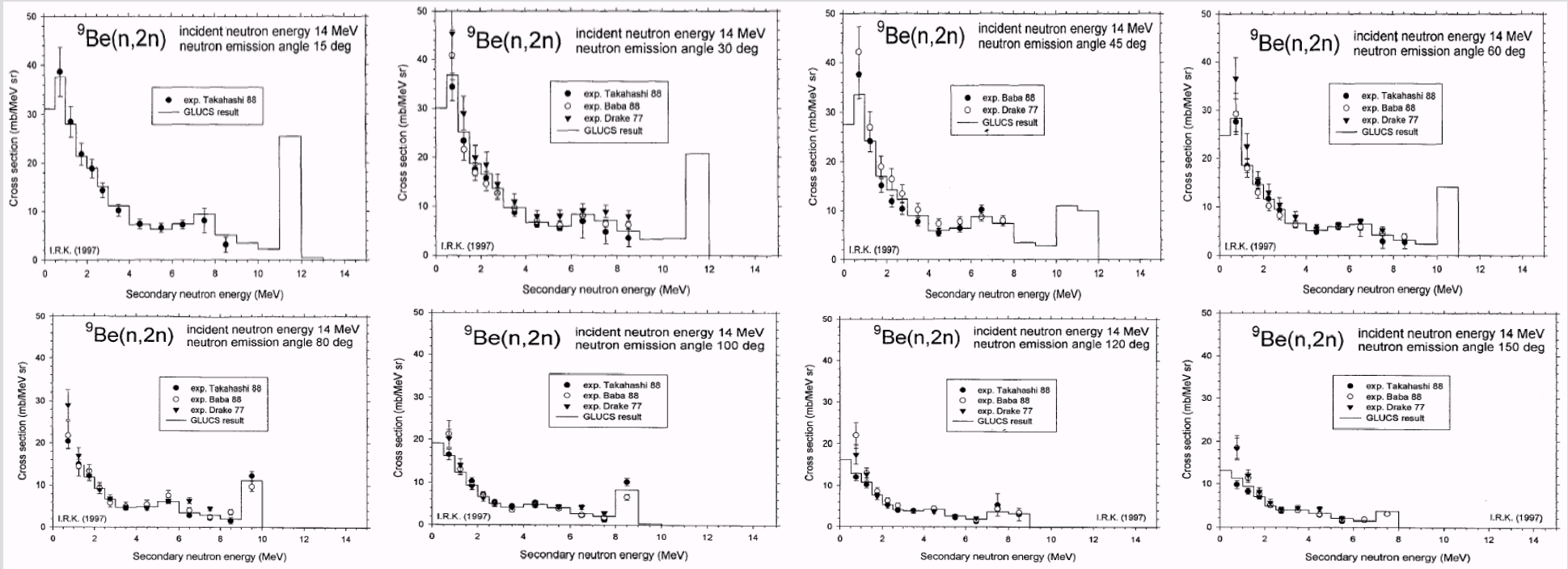
Top left: ^{9}Be(n,**n'n''**^{8}Be)

Top right: ^{9}Be(n,n_1'(α_o'(**n''**α")

Bottom left: ^{9}Be(n,n_1'(α_o'(**n''**α")

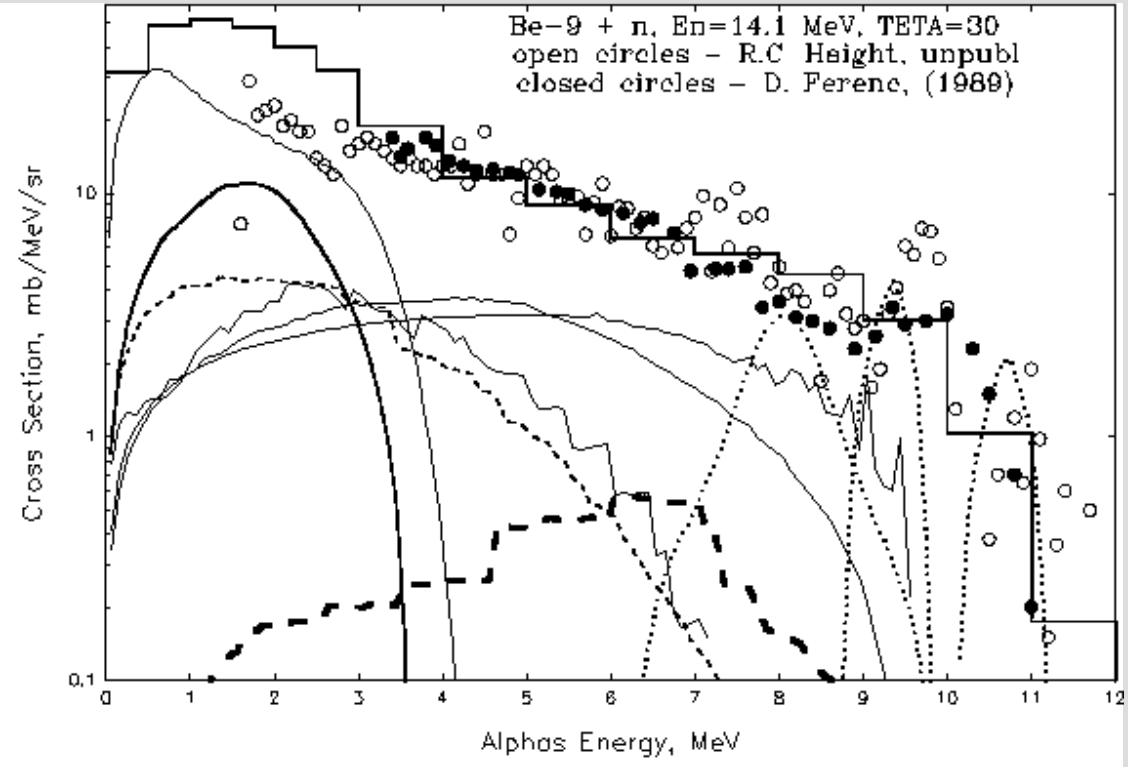
Bottom right: **Total neutron emission spectrum**

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions



Comparison of energy-angular distribution of **total neutron emission** for 14.1 MeV neutron incident energy. General agreement is good. Some lack of neutrons at low energies probably shows either the model of free kinematic break up used for some channels is not strict or problems with registration of neutrons with low energies at the experiment.

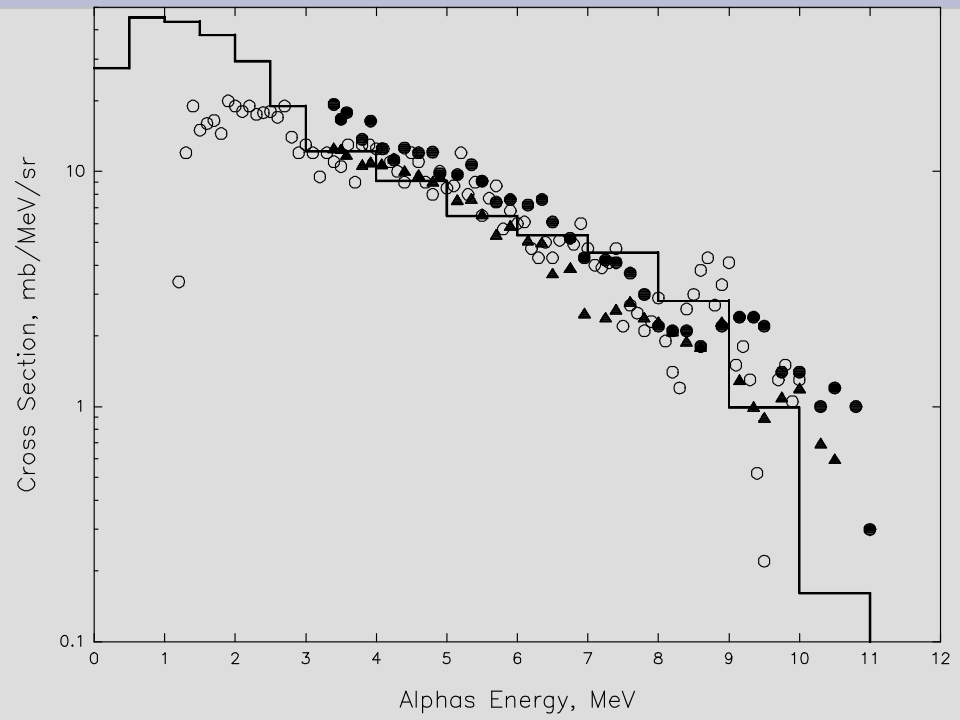
Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions

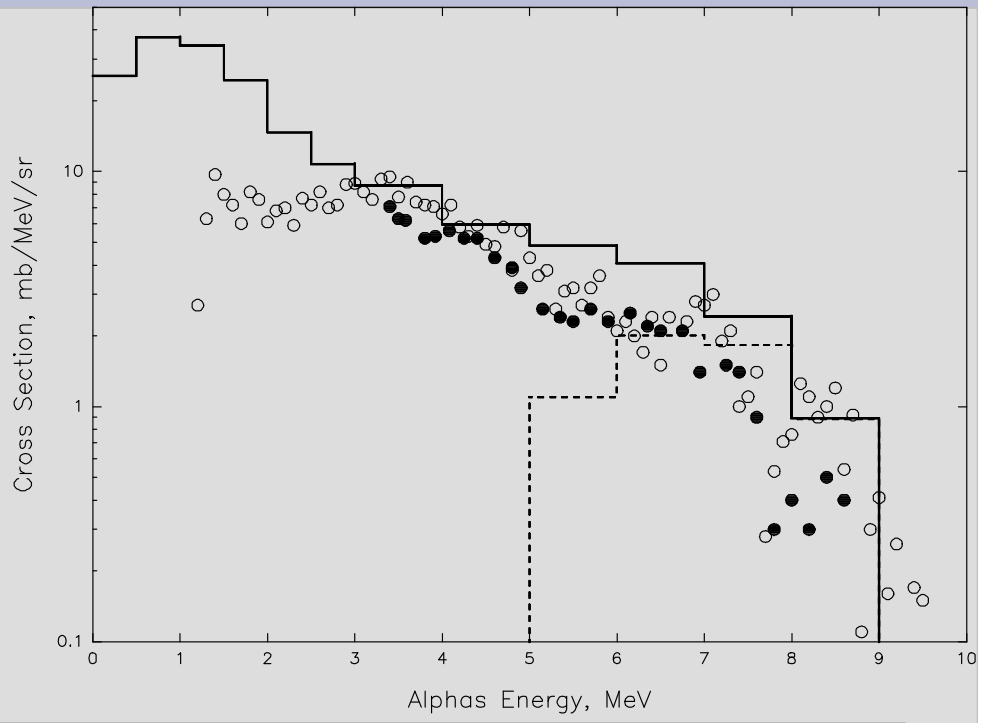


Good agreement for exclusion of low energies

Testing of the evaluation in the experiments with the measurements of **total a-particle emission** at 14.1 MeV neutron incident energy. Total evaluated spectrum is shown by histogram, with contribution of different channels: dotted lines – (n,α_0), (n,α_1), (n,α_2); two thin lines covering practically all spectrum- $(n,n\alpha'^{5}He)$ and $(n,n'a'(n''\alpha''))$; thin dashed line (below 7.3 MeV) – $(n, n'_7(\alpha_0'(n''\mathbf{a}'')))$; thin line (below 4.2 MeV) – $(n,n'_2(n''\alpha'\alpha'')$; thin broken line – $(n,n'n''(\alpha'\alpha''))$; thick dashed line – $(n,n'_7(n'_1(\alpha'\alpha'')))$; thick line – $(n,n'_{10}(\mathbf{a_0}'(n'\mathbf{a}'')))$.

Bayes approach to the description of the complex multi-step, multi-particle break-up processes in the case of ^{9}Be+n reactions





Comparison of the experimental data: left plate - by D. Ferenc (40 and 50 deg., closed circles and triangles) and R.C. Haight (45 deg., open circles) with evaluation for 45 deg. in the laboratory system; right plate - by D. Ferenc (90 deg., closed circles) and R.C. Haight (70 deg., open circles) with evaluation for 45 deg. in the laboratory system; dashed histogram shows contribution of (n,α_0), (n,α_1) and (n,α_2) channels. Excess of low-energy a-particles is observed

GMA code and simultaneous evaluation of neutron cross section standards, actinides cross sections and prompt fission neutron spectra

- GMA system was developed by **Wolfgang Poenitz** (ANL, USA) in the begin of 80-th.
- Used for non-model evaluation of the standard cross sections in the combined least-squares fit of related data.
- Includes 2 major codes DAT and GMA. DAT prepares input of experimental data (reducing of the data to chosen energy nodes using some prior data), GMA fits the data by least-squares method. Iteration procedure can be used for improving a prior data.
- Different reaction cross sections (not only the standards), their ratios and combinations and spectrum averaged cross sections can be used in the combined fit.

GMA code and sim ultaneous evaluat ion of standards and actinides n eutron cross sections and prompt fission neutron spectra

The code allows account the following types of the data:

- absolute cross section measurements (measurements of total cross sections by transmission method, measurements with the associated particles method, measurements relative «absolute standard» - $^{1}H(n,p)$ cross section)
- sum of absolute cross sections and combinations which include ratio of absolute cross section to the sum of other absolute cross sections
- measurements of the shape of the cross section (non-normalized cross sections)
- ratio of absolute cross sections (absolute ratios)
- ratios of the shapes of the cross sections (non-normalized ratios, shape of the ratios)
- integrals on given spectrum (spectrum averaged cross sections, in particular — prompt fission neutron spectrum of $^{252}Cf(sf)$, which is standard).

GMA code and sim ultaneous evaluat ion of standards and actinides n eutron cross sections and prompt fission neutron spectra

The code allows account the SERC, LERC and MERC types of uncertainties as well as correlations between different data sets.

At present length of the data vector is limited by 1200 data, what corresponds maximum size of covariance matrix 1200*1200.

Standards database used in the fit, at present includes more than 430 experimental data sets covering the energy range between thermal point and 200 MeV.

GMA code and sim ultaneous evaluat ion of standards and actinides n eutron cross sections and prompt fission neutron spectra

	^{6}Li(n,α)	^{10}B(n,α$_0$)	^{10}B(n,α$_1$)	^{10}B(n,α)	Au(n,γ)	^{238}U(n,γ)	^{235}U(n,f)	^{239}Pu(n,f)	^{238}U(n,f)
^{6}Li(n,α)	18 (7)								
^{10}B(n,α$_0$)	0	5 (4)							
^{10}B(n,α$_1$)	1 (0)	12 (10)	11 (2)						
^{10}B(n,α)	4 (0)	0	0	5 (2)					
Au(n,γ)	3 (3)	0	6 (3)	4 (4)	27 (21)				
^{238}U(n,γ)	2 (2)	0	9 (5)	4 (4)	10 (9)	14 (11)			
^{235}U(n,f)	14 (0)	0	2 (1)	25 (0)	12 (10)	12 (6)	68 (52)		
^{239}Pu(n,f)	2 (0)	0	0	19(0)	0	1 (0)	19 (14)	22 (19)	
^{238}U(n,f)	2 (1)	0	0	0	0	0	34 (29)	3 (1)	18 (11)

- Experimental data sets for standards evaluation: on diagonal – for given cross section, off-diagonal – for ratios of cross sections; numbers – numbers of data sets including for ratios given in brackets.
- Data sets not shown – total and elastic scattering for ^{7}Li and ^{10}B used as constraints and 26 pre-evaluated thermal constants.

GMA code and sim ultaneous evaluat ion of standards and actinides n eutron cross sections and prompt fission neutron spectra

```
3581966AU(N,G)                  W.P.POENITZ                  JNEA/B20,825(1967)
1 1 0 0  9    1  6  0  0  0  0
UNCERTAINTIES
1 EFFICIENCY RATIO
2 AU DECAY
3 BE DECAY
4 NEUTRON SELFSHIELDING + SCATTERING
5 GAMMA ABSORPTION
6 TIME FACTORS
7 NEUTRON ATT. +SCATT. FROM TARGET
RENORM TO CURRENT BE-7 BRANCHING
   .8   .3   .5   .5   .5   .4   .3   .0   .0   .0  1  1  1  1  1  1  1  0  0  0
  .00  .00  .00
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  .00  .00  .00
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  .50  .50  .50
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 .3000E-01 .6005E+00   .0 23.0   .8   .0   .0   .0   .0   .0   .0   .0   .0  1.5
ESESESESES
```

Data set 358

Example of DAT input of 3 data set (358, 359 and 360) with correlations: 358 and 359 - 100% in the correction at neutron self-shielding and scattering in the samples 100 % in the correction at neutron attenuation and scattering in the target; Between uncertainties of the data in the data set 360 and data sets 358 and 359 there are 100 % correlations in the uncertainty of the correction at neutron self-shielding and scattering in the samples

GMA code and sim ultaneous evaluat ion of standards and actinides n eutron cross sections and prompt fission neutron spectra

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 3591966AU(N,G)                 W.P.POENITZ                JNEA/B20,825(1967)
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 UNCERTAINTIES
 1 AU DET. EFF.
 2 MN DET. EFF.
 3 AU MASS
 4 TIME FACTORS
 3 STATISTICS
 4 LEAKAGE
 5 SELFSHIELDING + SCATTERING
 6 ATT. + SCATTERING IN TARGET
 7 CAPTURE IN CHANNEL
   .8   .8   .1   .5   .0   .0   .0   .0   .0   .0  1  1  1  1  0  0  0  0  0  0
  .00  .00  .00
  .00  .00  .00
  .00  .00  .00
  .50  .50  .50
  .30  .70  .20
  .50  .50  .50
  .50  .50  .50
  .00  .00  .00
  .00  .00  .00
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 .6400E-01 .3600E+00   .0 15.0   .0  1.4   .3   .4   .2   .0   .0   .0  5.7  1.9
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Data set 359

GMA code and sim ultaneous evaluat ion of standards and actinides n eutron cross sections and prompt fission neutron spectra

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 4 NEUTR. DET. EFF.
 5 SELFSHIELDING + SCATTERING
 6 GAMMMA DET. EFF.
 7 GAMMA DET. BIAS + ENERGYDET.
 8 GREY NEUTRON DET. EFF.
 9 GREY NEUTR. DET. ANISOTROPY
 10 BACKGROUND
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  .00  .00  .00
  .00  .00  .00
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  .50  .50  .50
  .50  .50  .50
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  .50  .50  .50
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 .2500E-01 .6224E+00  3.6  8.0  3.9   .1  2.0   .1  1.0  1.0   .1  1.0   .0  4.7
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 ................missed lines.....................................................
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 .4730E+00 .1374E+00  2.1  8.0  1.1   .7  1.1  3.8  1.2  2.0  1.9  1.9   .0  5.5
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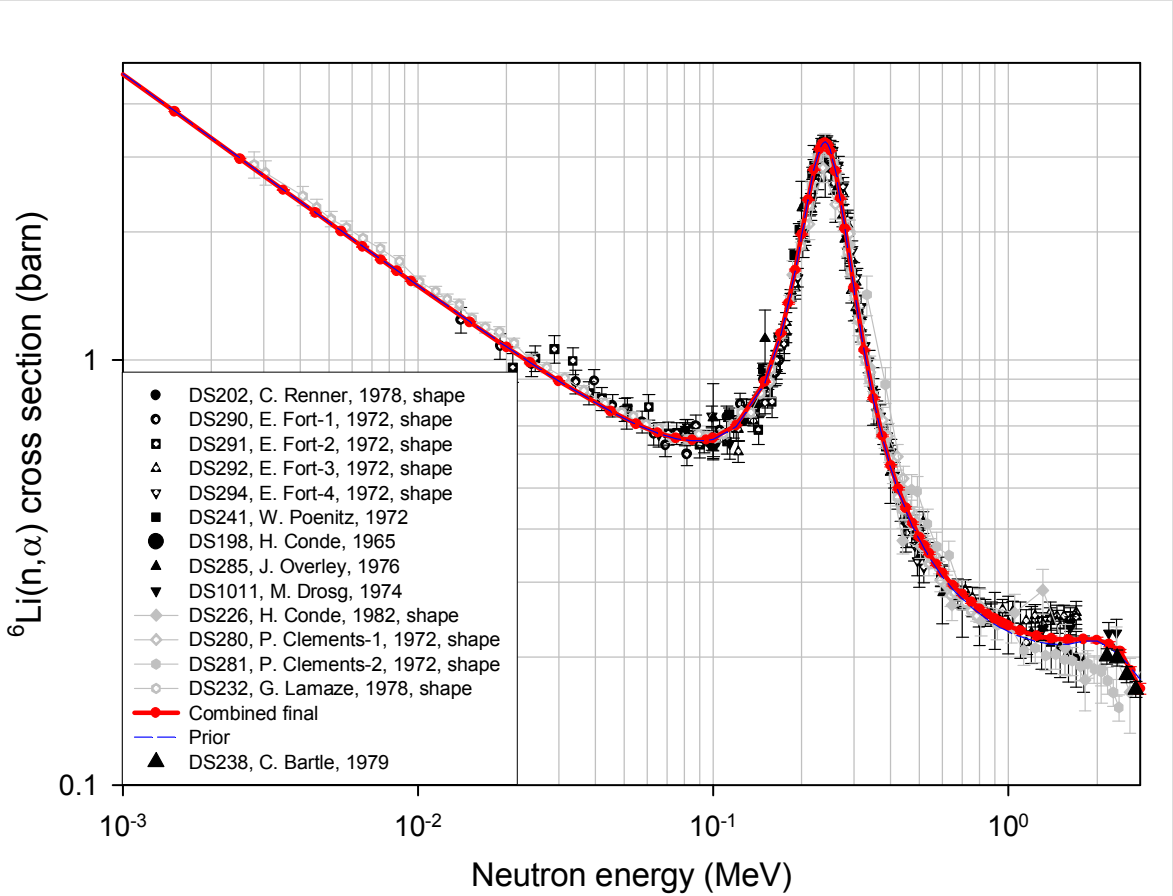
Data set 360

GMA code and sim ultaneous evaluat ion of standards and actinides n eutron cross sections and prompt fission neutron spectra

Combined (simultaneous) evaluation of the standards was done:

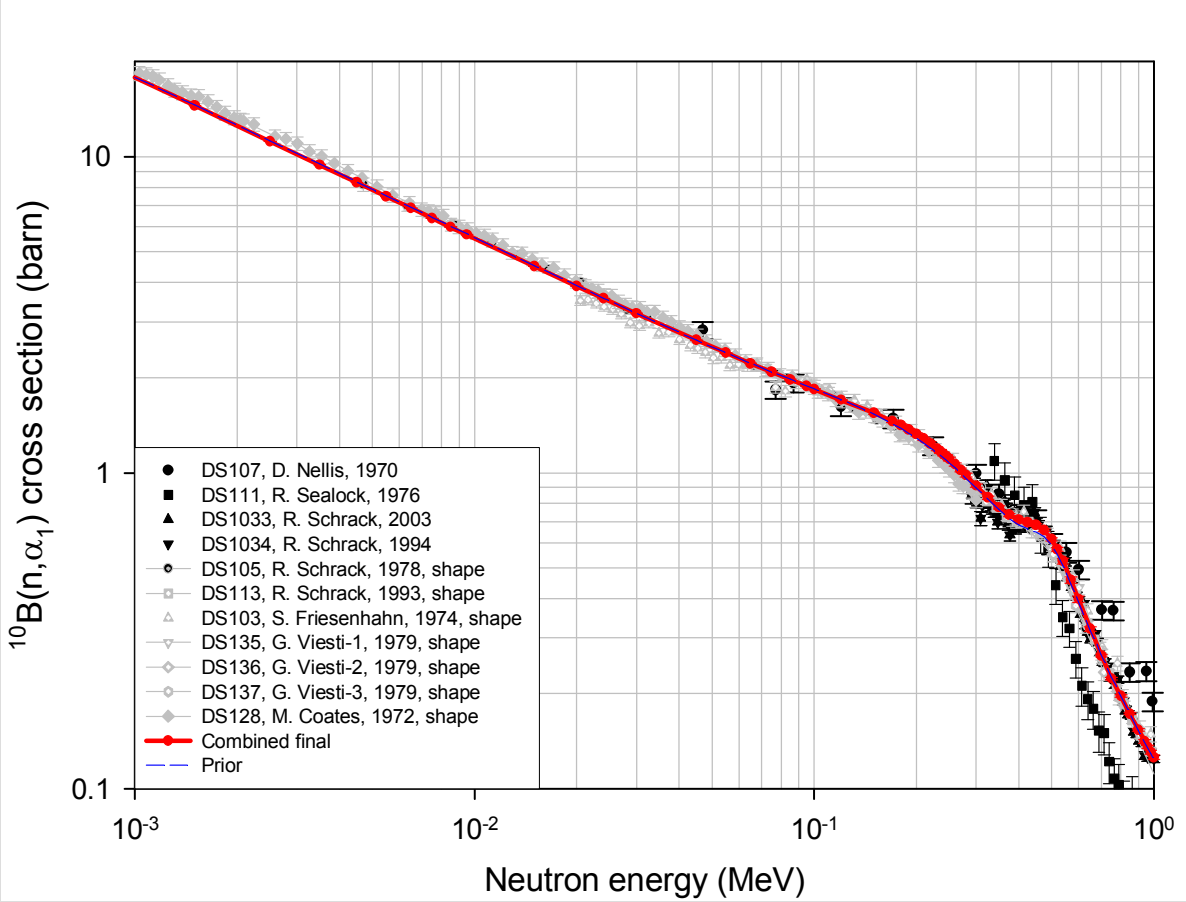
- with inclusion of thermal constants pre-evaluated by Axton and adding of new high-precision experimental data obtained after Axton evaluation
- with independent evaluation of ^{6}Li(n,t) and ^{10}B(n,α_0), ^{10}B(n,α_1) cross section in the R-matrix model (EDA and RAC codes) and inclusion of these evaluations as pseudo-experimental data sets together with other experimental data not used in the R-matrix fit in the combined fit of all standards
- with experimental data reduced to the initial form obtained by the authors
- with outlying data analysed and with introducing of additional MERC type uncertainty to this data leading to the final χ^2 per degree of freedom of the order 1.

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



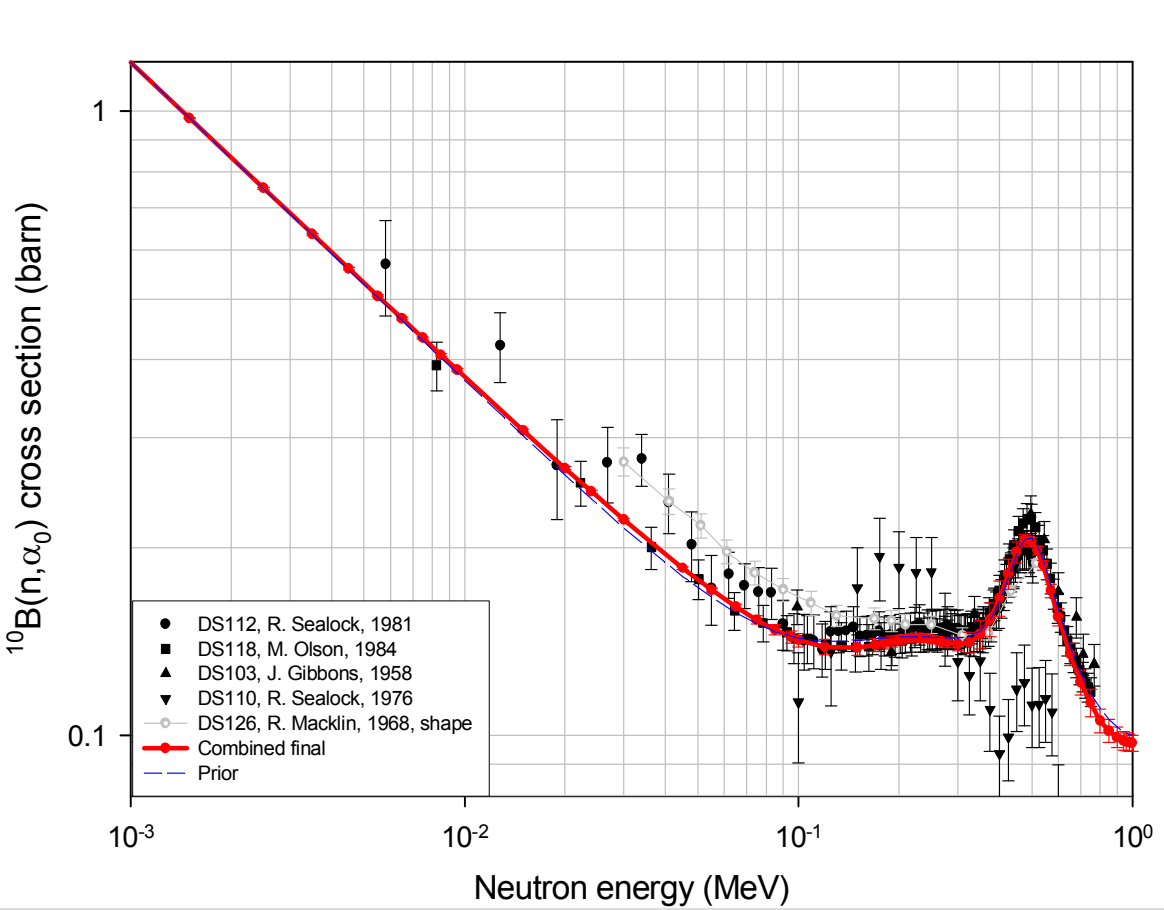
Cross section of the ^{6}Li(n,t)α reaction

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



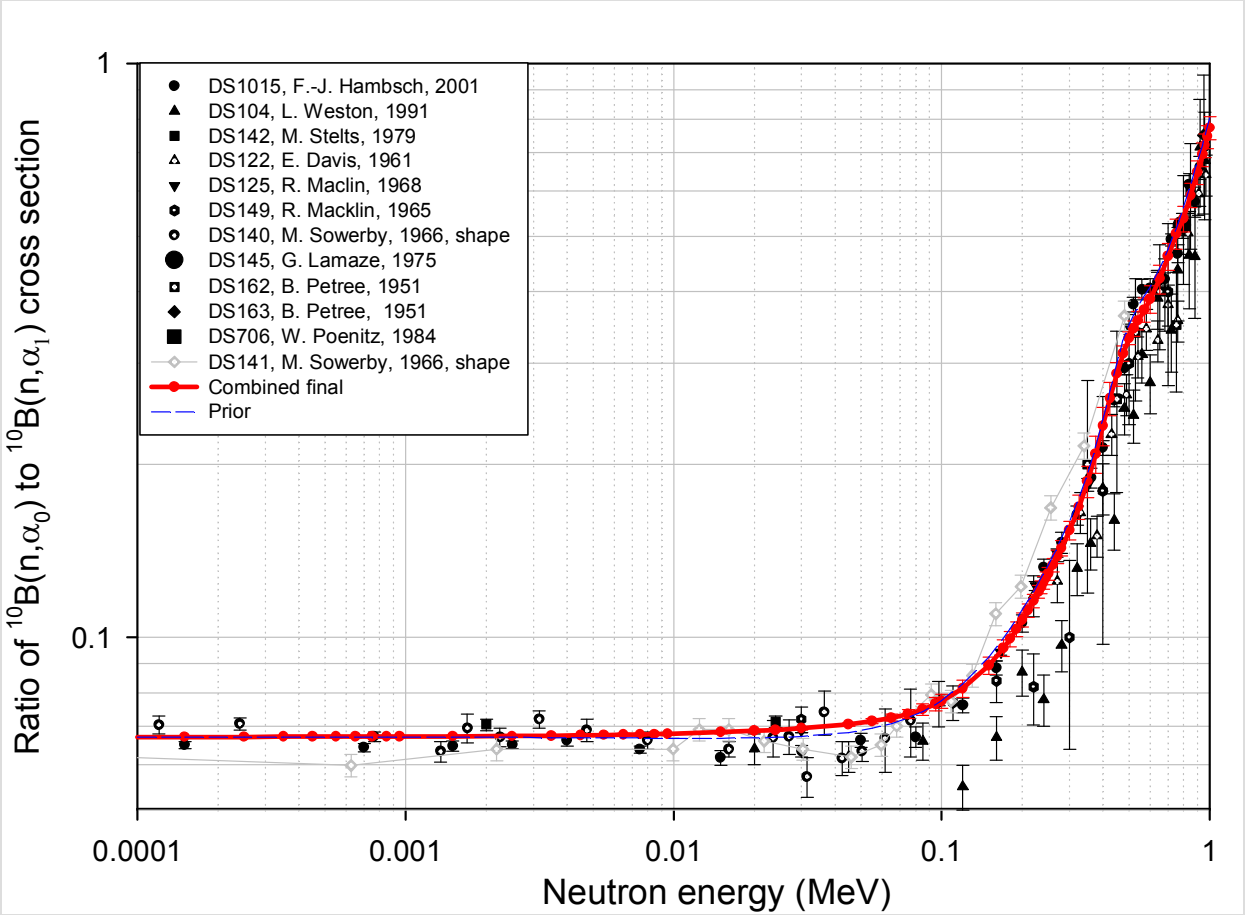
Cross section of $^{10}B(n,\alpha_1)$ reaction.

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



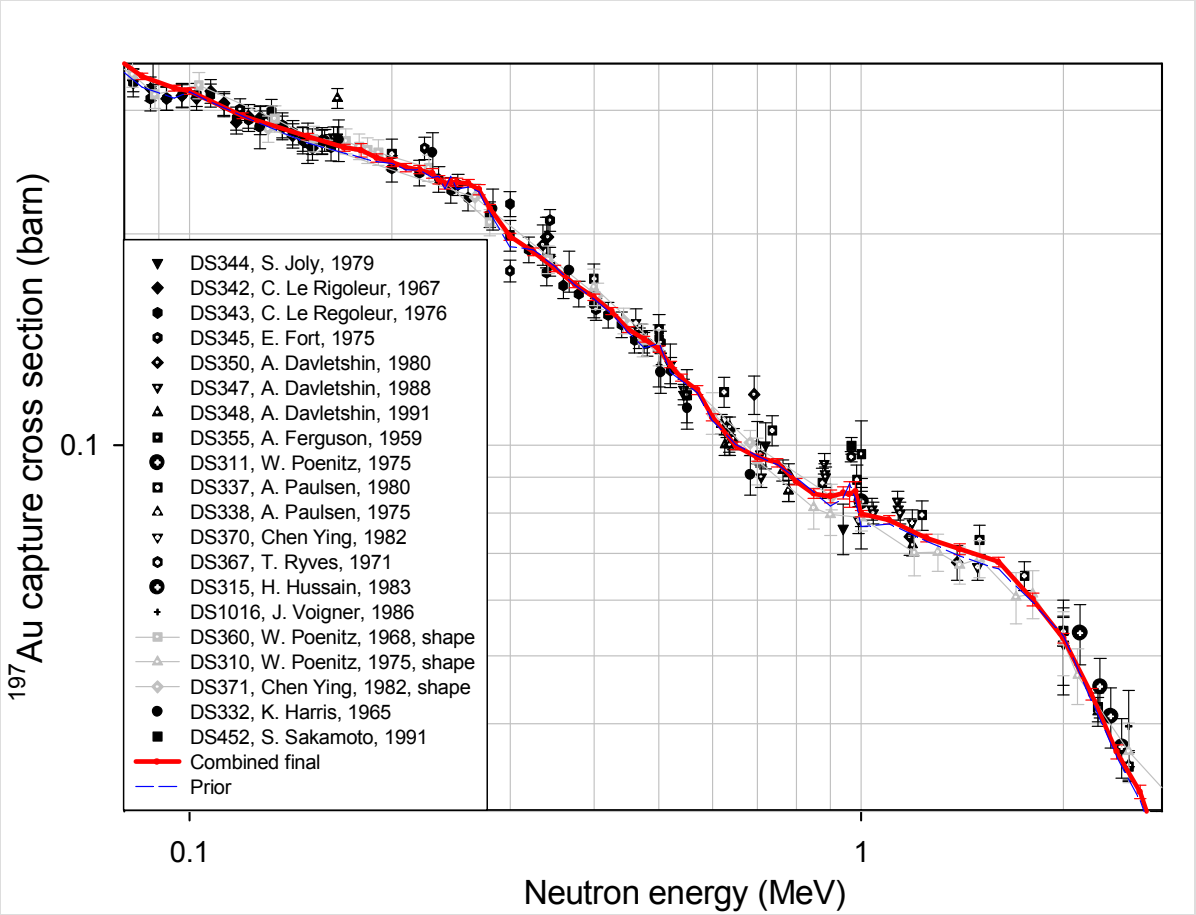
Cross section of ^{10}B(n,α_0) reaction.

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



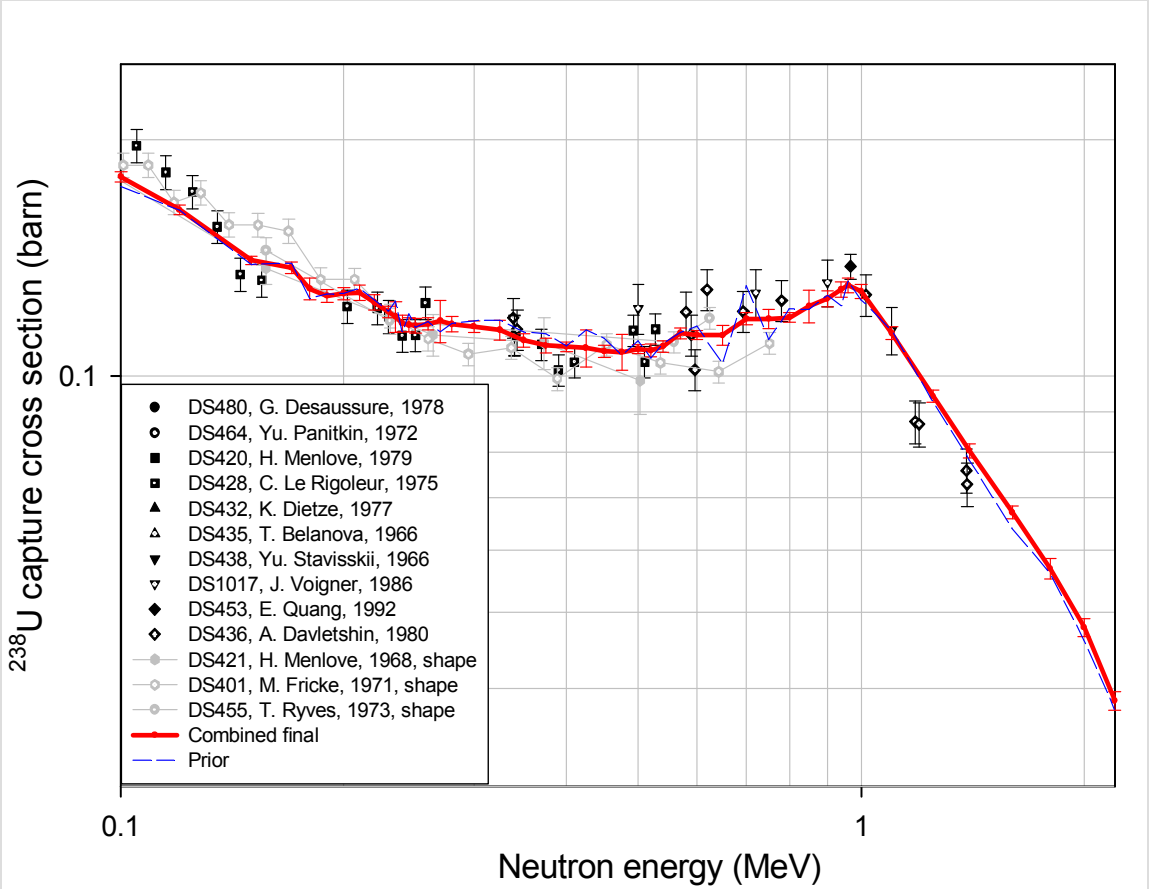
Ratio of the cross sections of $^{10}B(n,\alpha_0)$ to $^{10}B(n,\alpha_1)$ reaction.

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



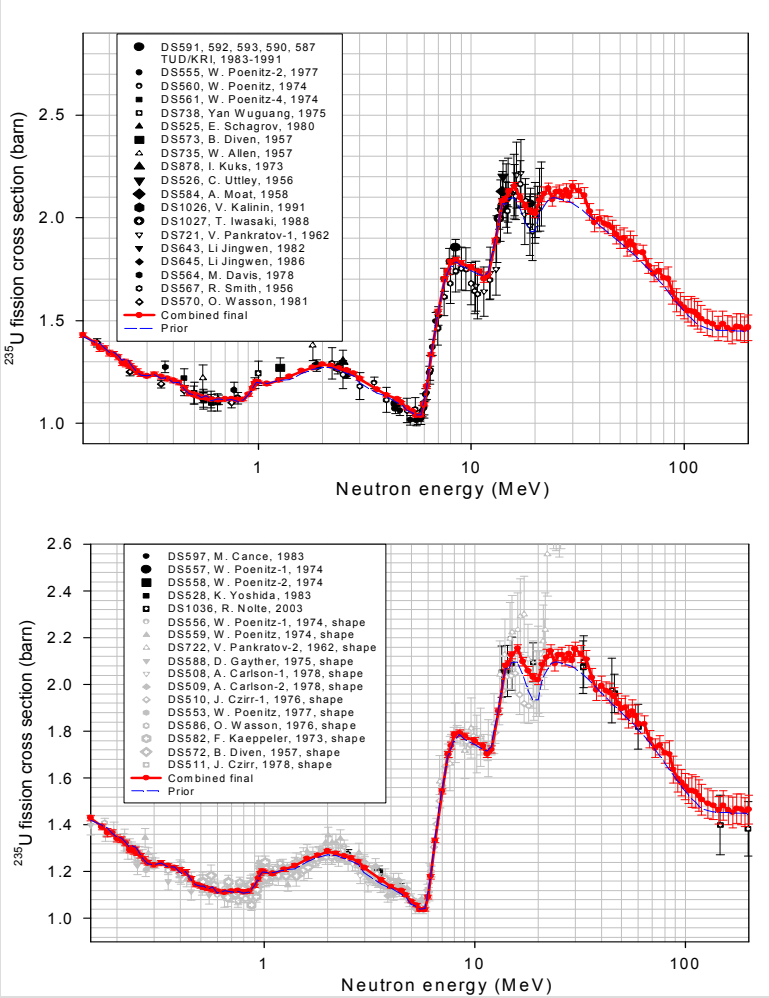
Cross section of the ^{197}Au(n,γ) reaction.

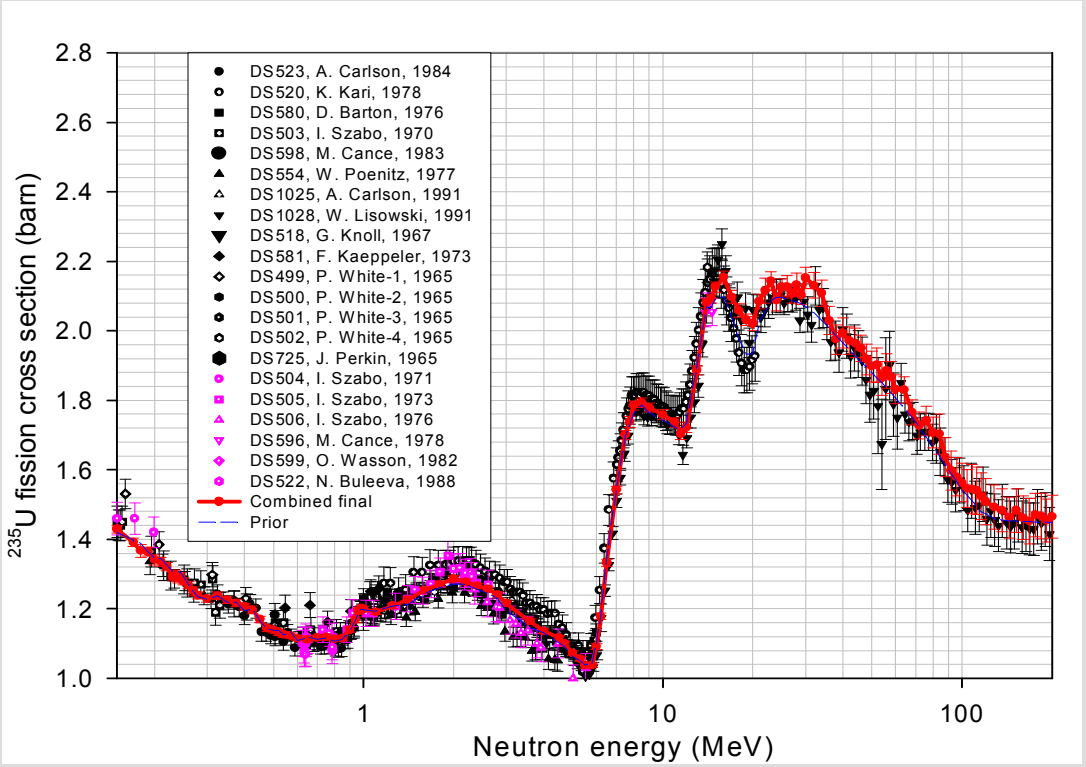
GMA code and sim ultaneous evaluat ion of standards: results of evaluation



Cross section of ^{238}U(n,γ) reaction.

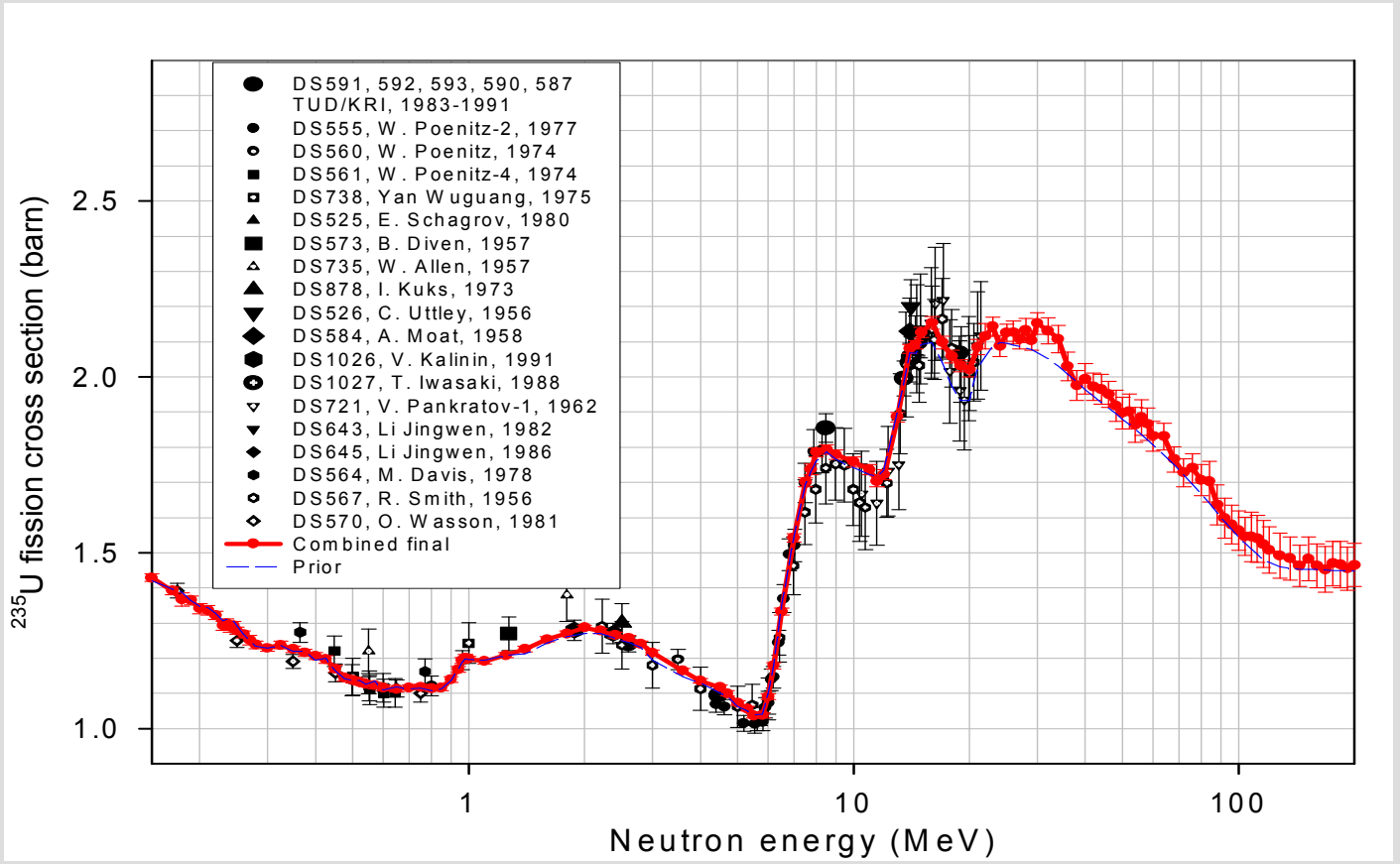
GMA code and sim ultaneous evaluat ion of standards: results of evaluation





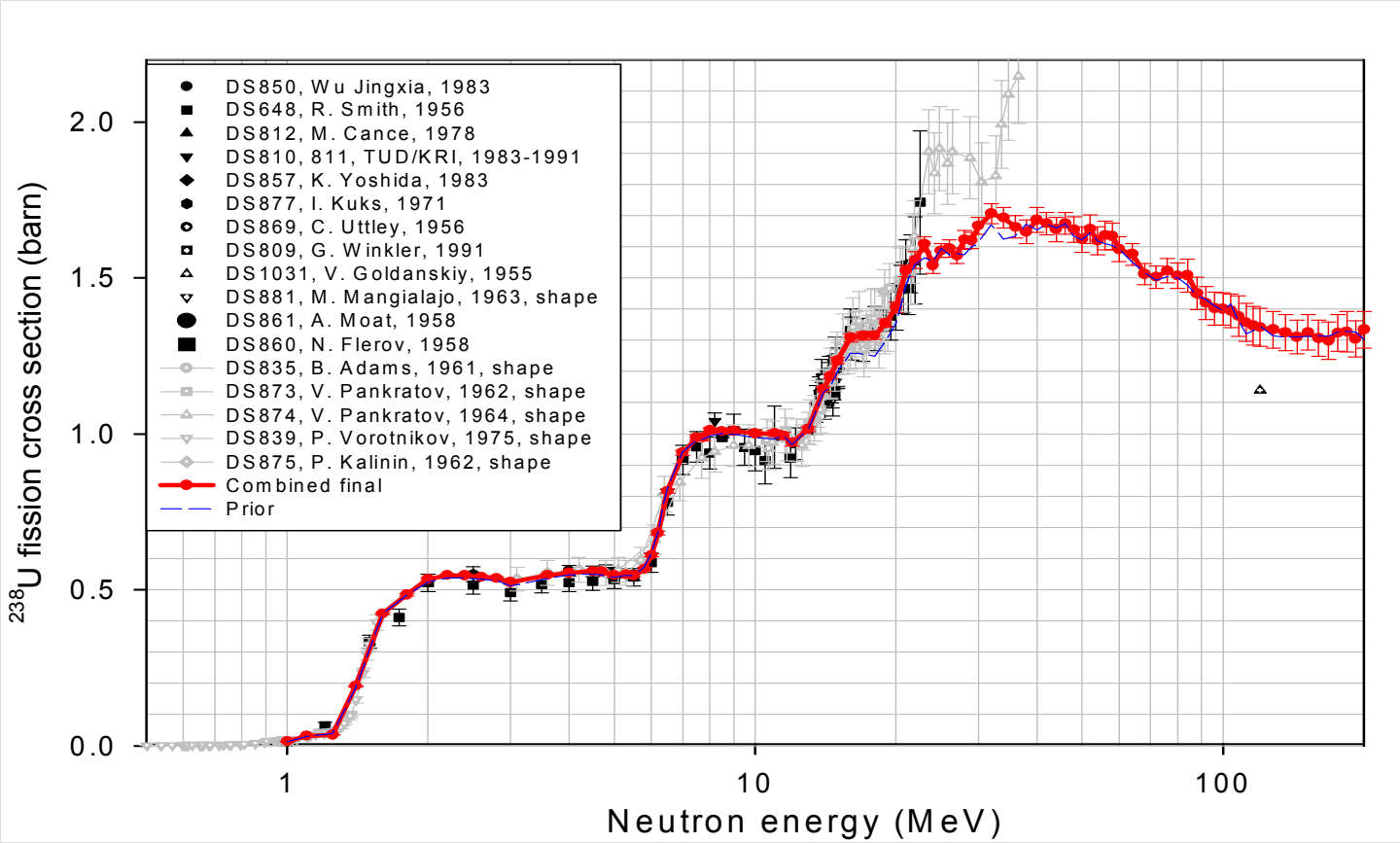
Cross section of $^{235}U(n,f)$ reaction with large number of experimental data.

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



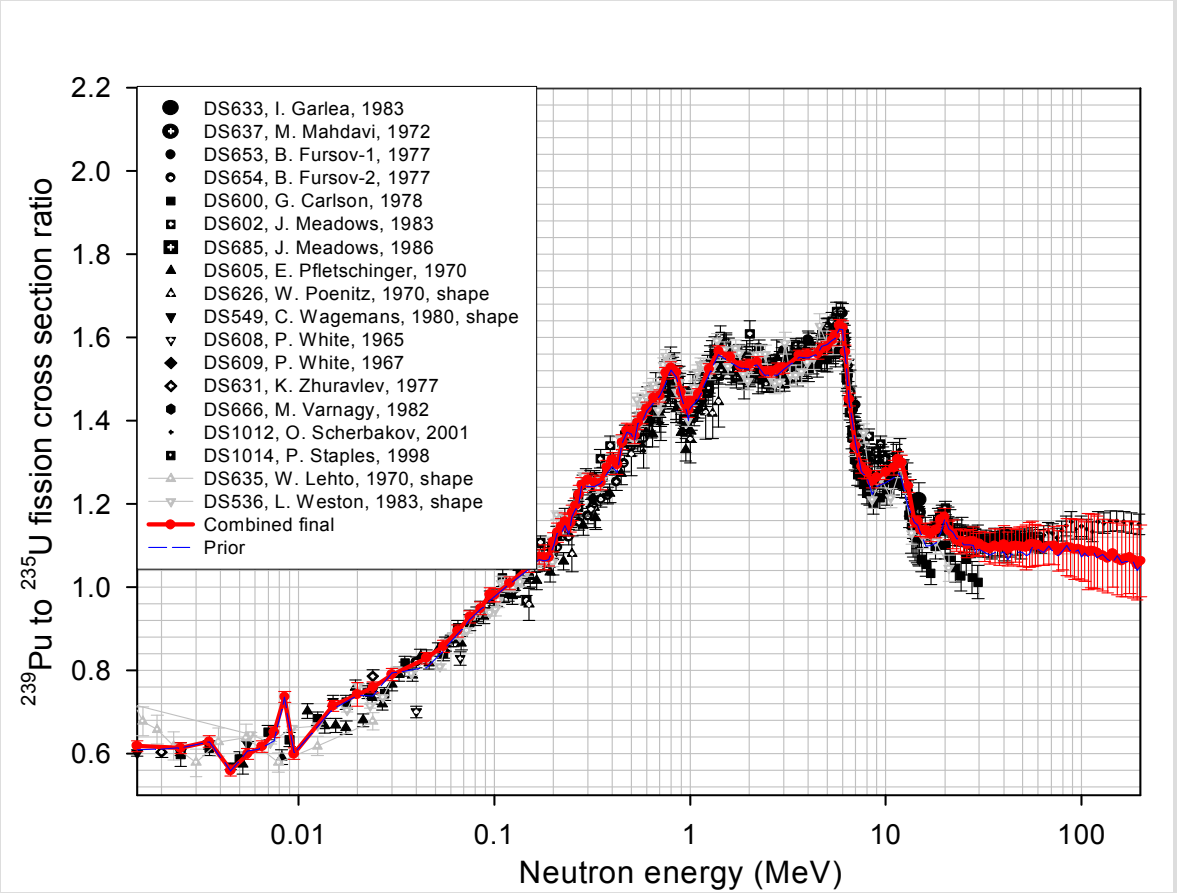
Cross section of ^{239}Pu(n,f) reaction.

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



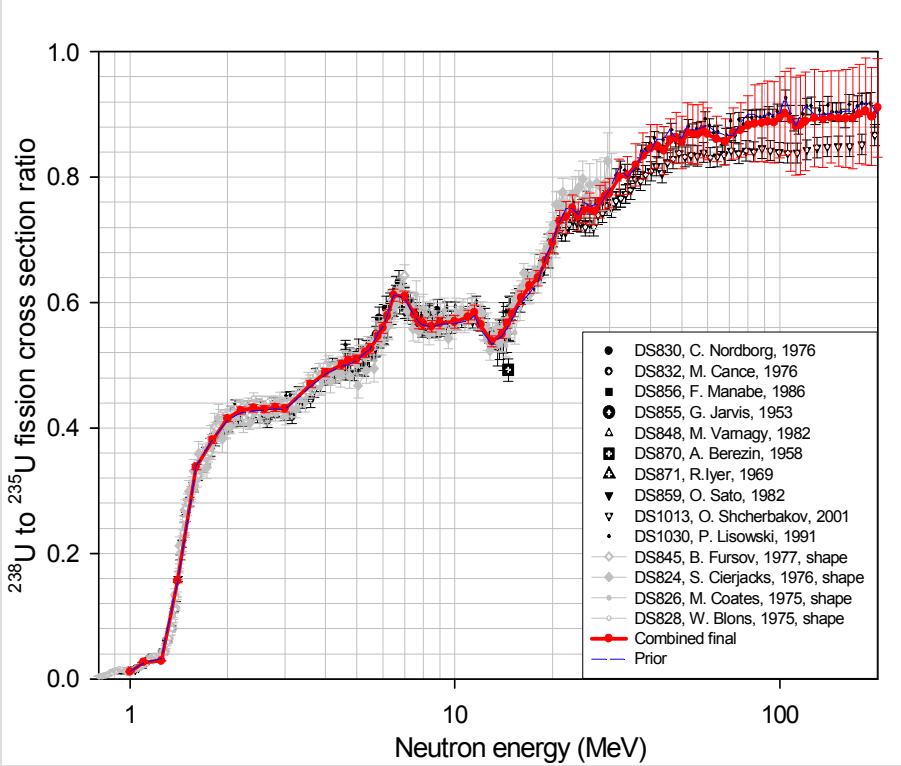
Cross section of ^{238}U(n,f) reaction.

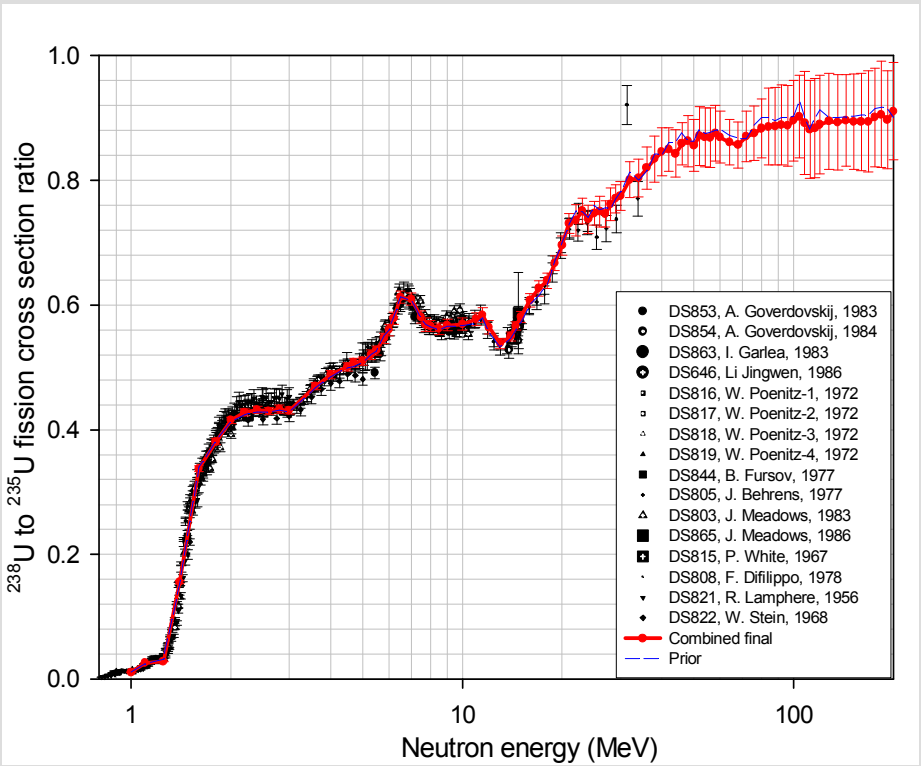
GMA code and sim ultaneous evaluat ion of standards: results of evaluation



Ratio of the cross sections of ^{239}Pu(n,f) to ^{235}U(n,f) reaction

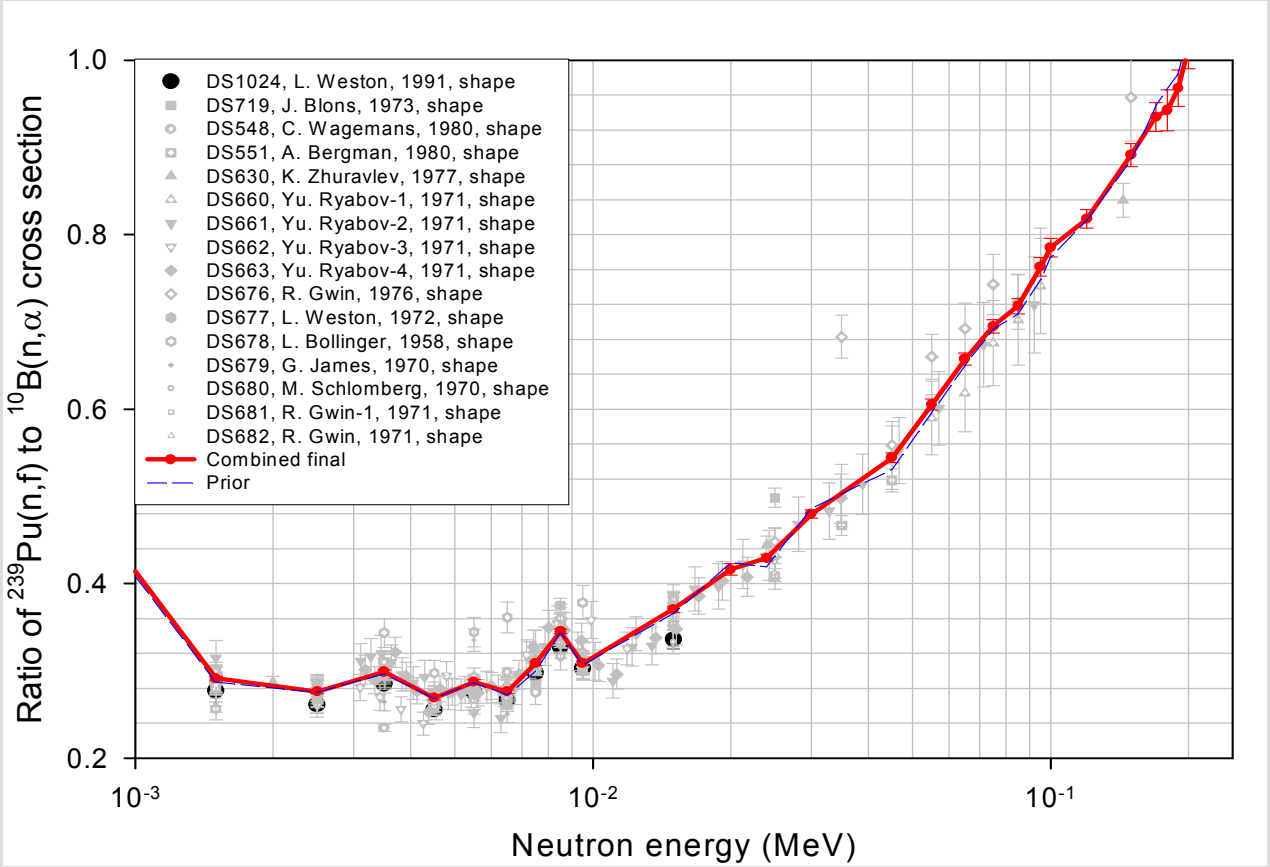
GMA code and sim ultaneous evaluat ion of standards: results of evaluation





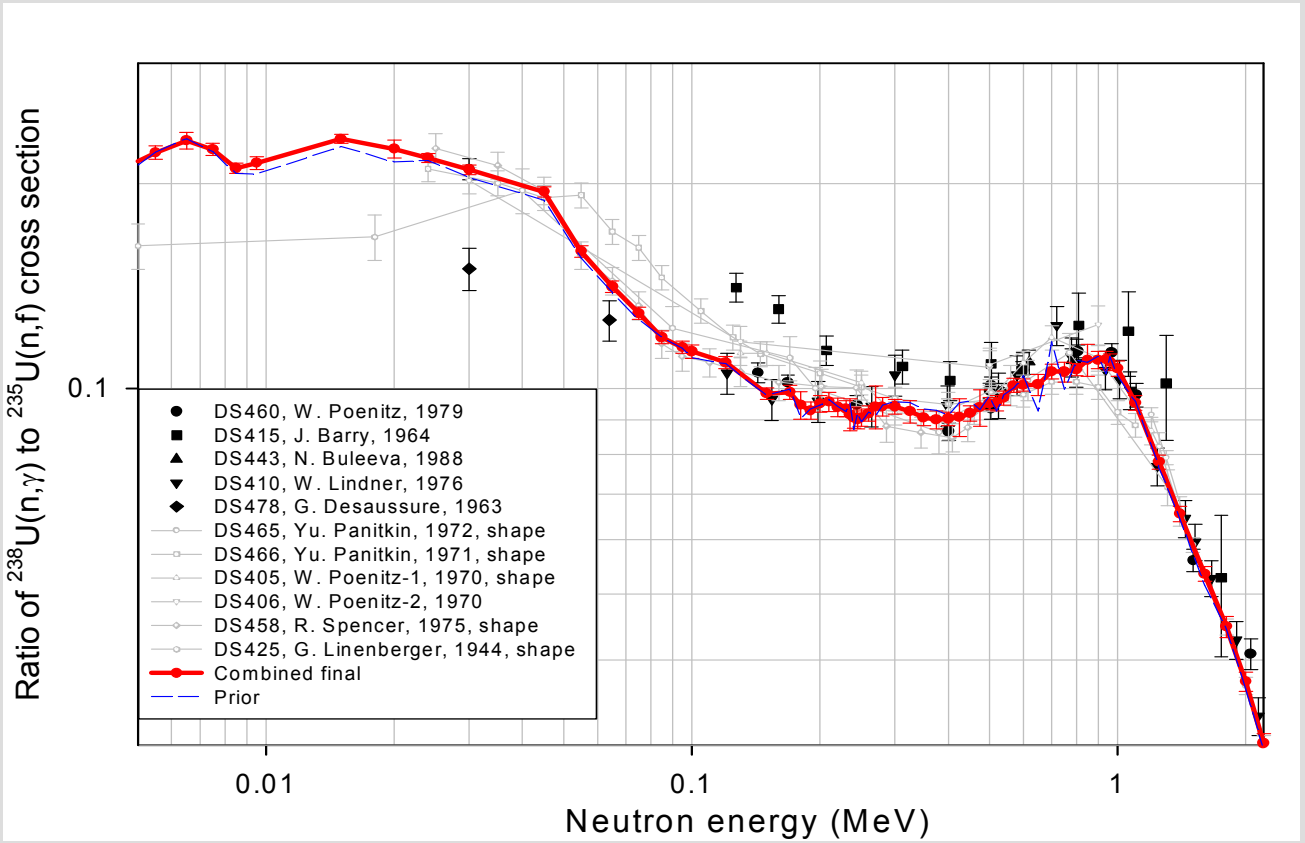
Ratio of the cross sections of ^{238}U(n,f) to ^{235}U(n,f) reaction.

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



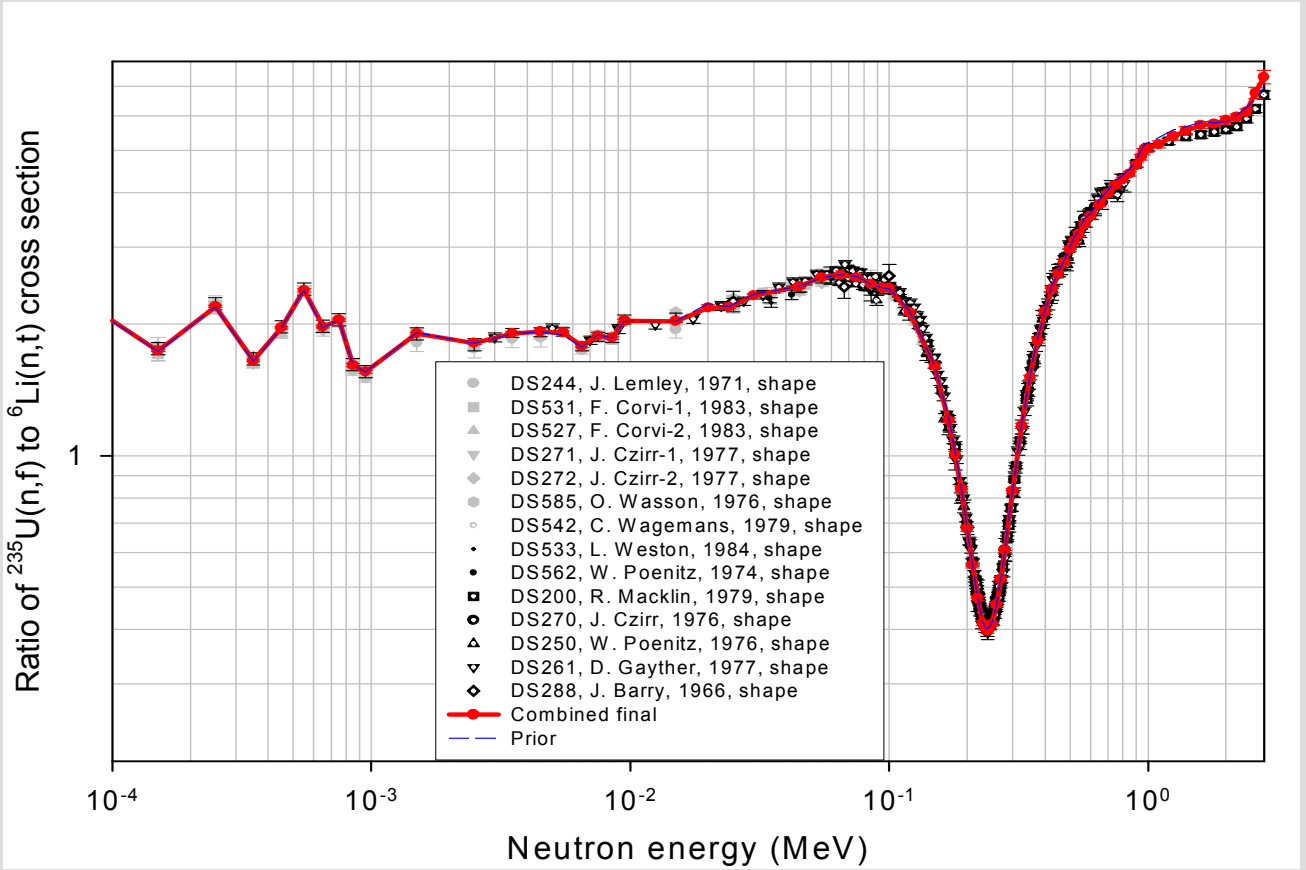
Ratio of the cross sections of ^{239}Pu(n,f) to ^{10}B(n,α) reaction.

GMA code and sim ultaneous evaluat ion of standards: results of evaluation



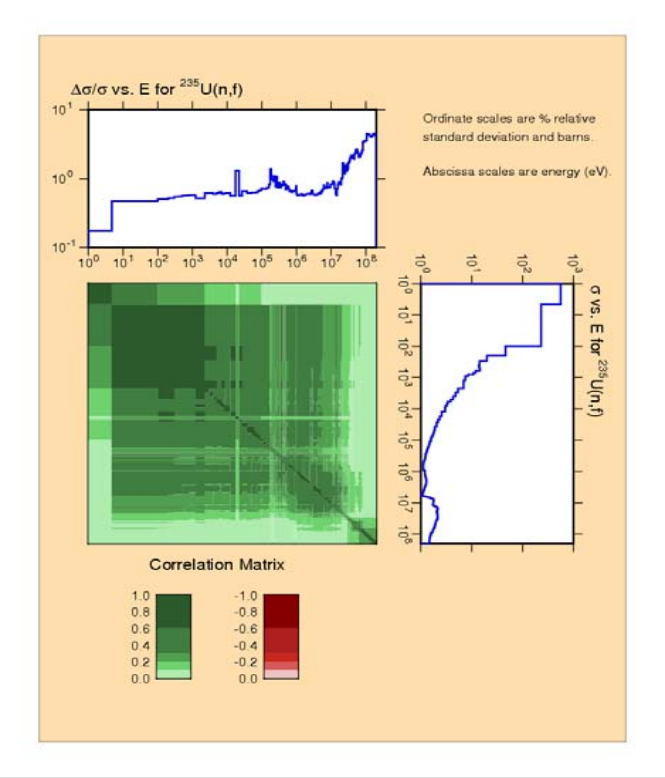
Ratio of the cross sections of ^{238}U(n,γ) to ^{235}U(n,f) reaction.

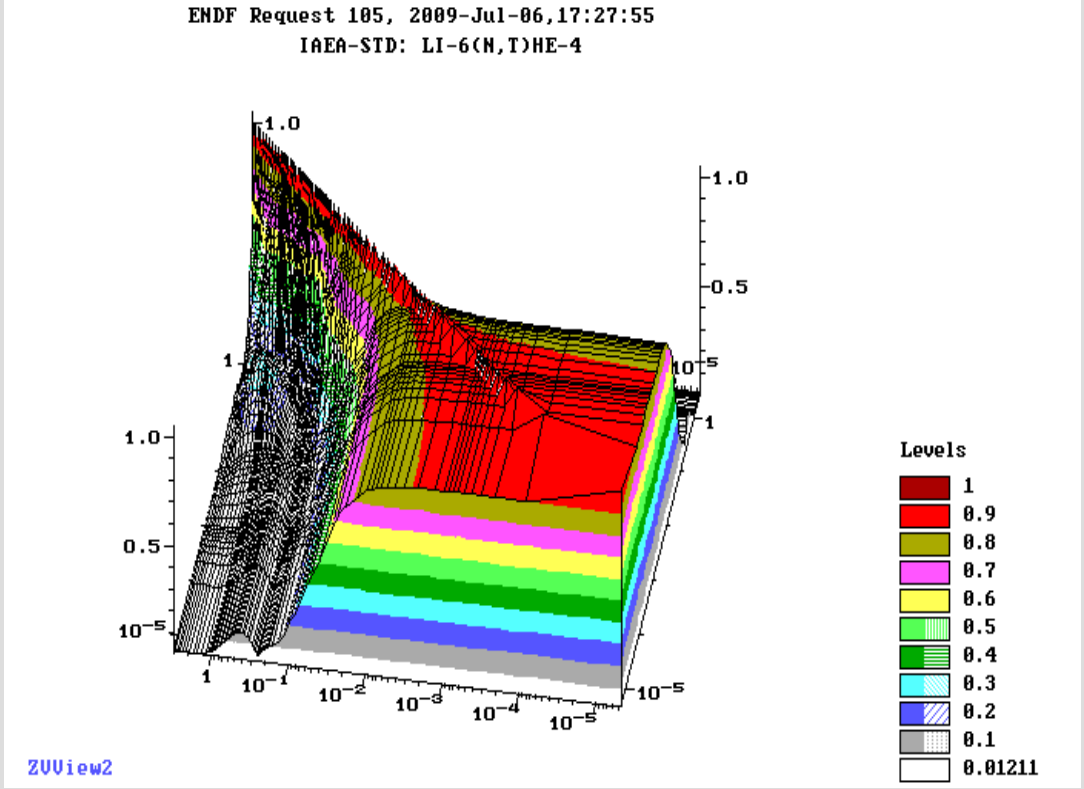
GMA code and sim ultaneous evaluat ion of standards: results of evaluation



Ratio of the cross sections of ^{235}U(n,f) to ^{6}Li(n,t) reaction.

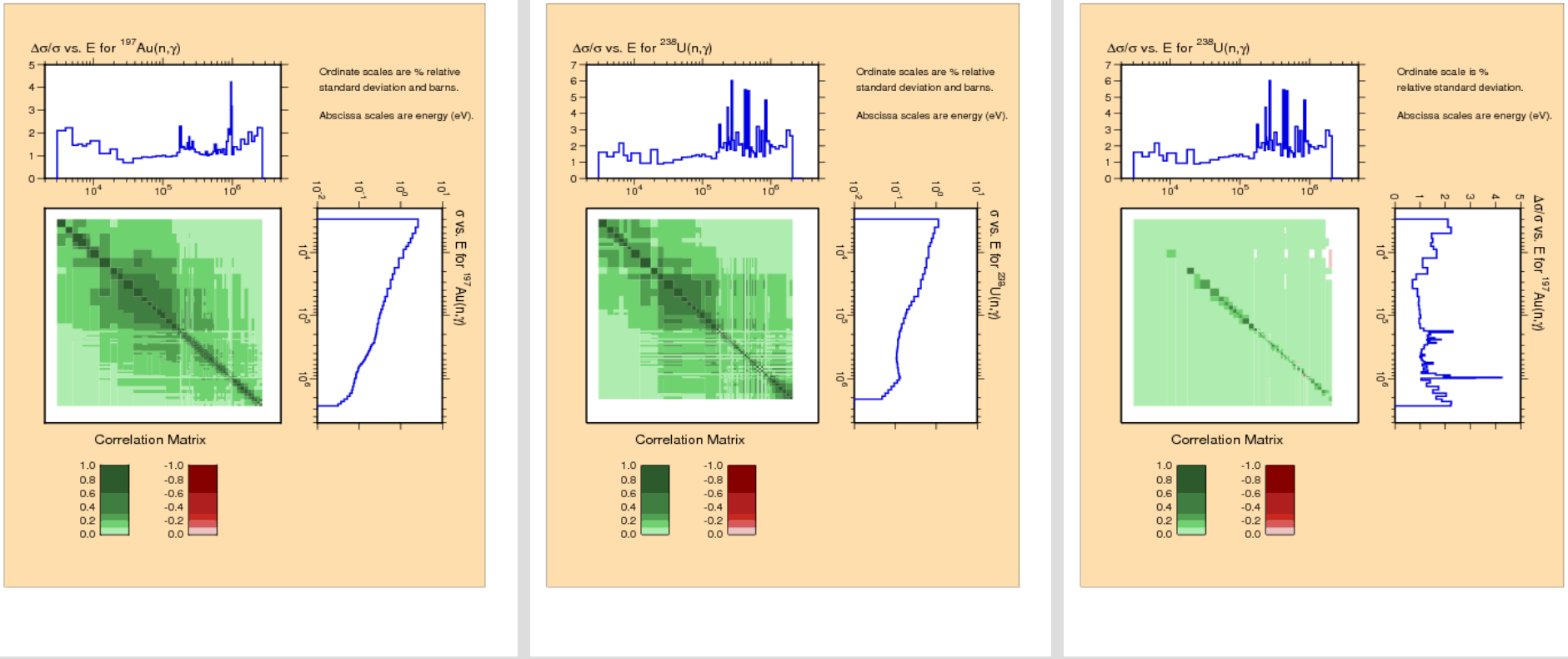
GMA code and sim ultaneous evaluat ion of standards: result s of evaluat ion (correlation matrices)





Correlation matrices of uncertainties : NJOY style - left figure, for ^{235}U(n,f); 3 – dimensional presentation in the development by V. Zerkin – right figure, for ^{6}Li(n,t) reaction

GMA code and sim ultaneous evaluat ion of standards: result s of evaluat ion (correlation matrices)



Three blocks of full correlation matrix of the uncertainties of the ^{197}Au(n,γ) and ^{238}U(n,γ) cross sections.

GMA code and sim ultaneous evaluat ion of standards and minor actinides

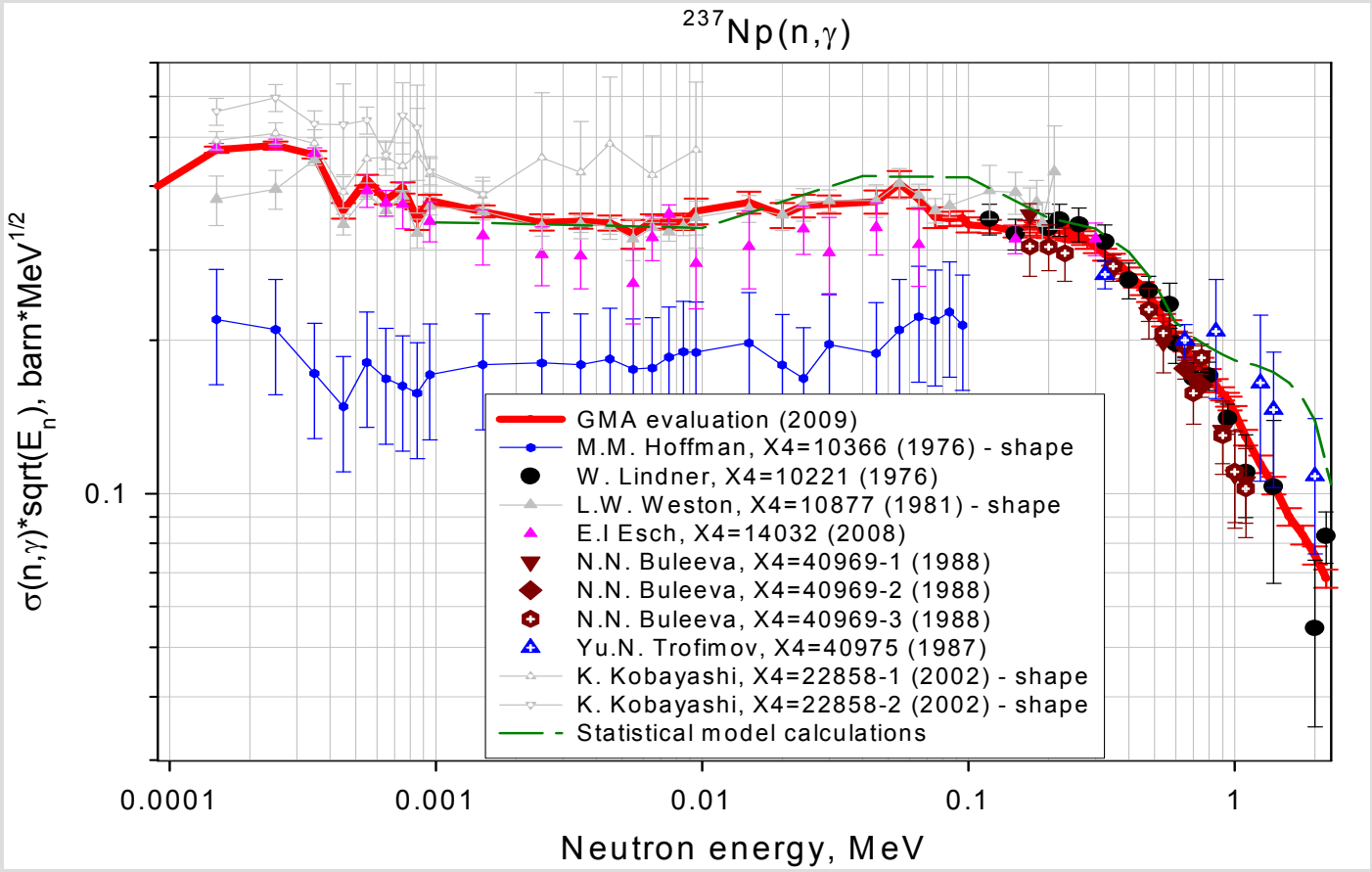
• Evaluation of the fission and capture cross sections of minor actinides important for the fuel cycle closing tasks can be done with the evaluated standards and their full covariance matrix of the uncertainties:

➔ (a) either with addition of the minor actinides experimental data to the standards experimental data base and the following combined evaluation,

➔ (b) or in the Bayesian approach, when minor actinides data are fitted together with the evaluated standards introduced in the GMA as large pseudo-experimental data set.

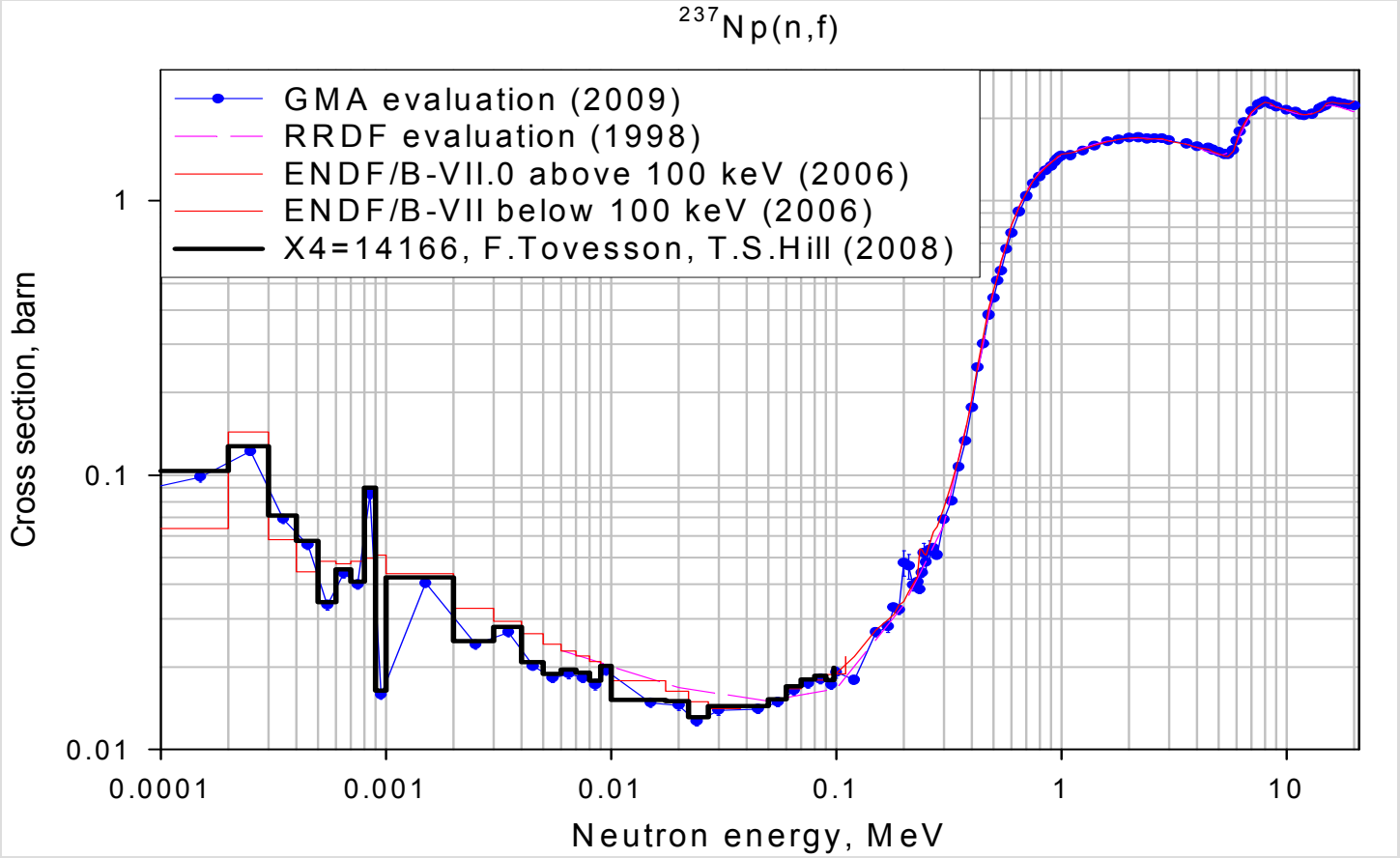
(a) was used for evaluation of ^{237}Np(n,γ) and ^{237}Np(n,f) cross section (combined fit all standards).

GMA code and sim ultaneous evaluat ion of standards and minor actinides



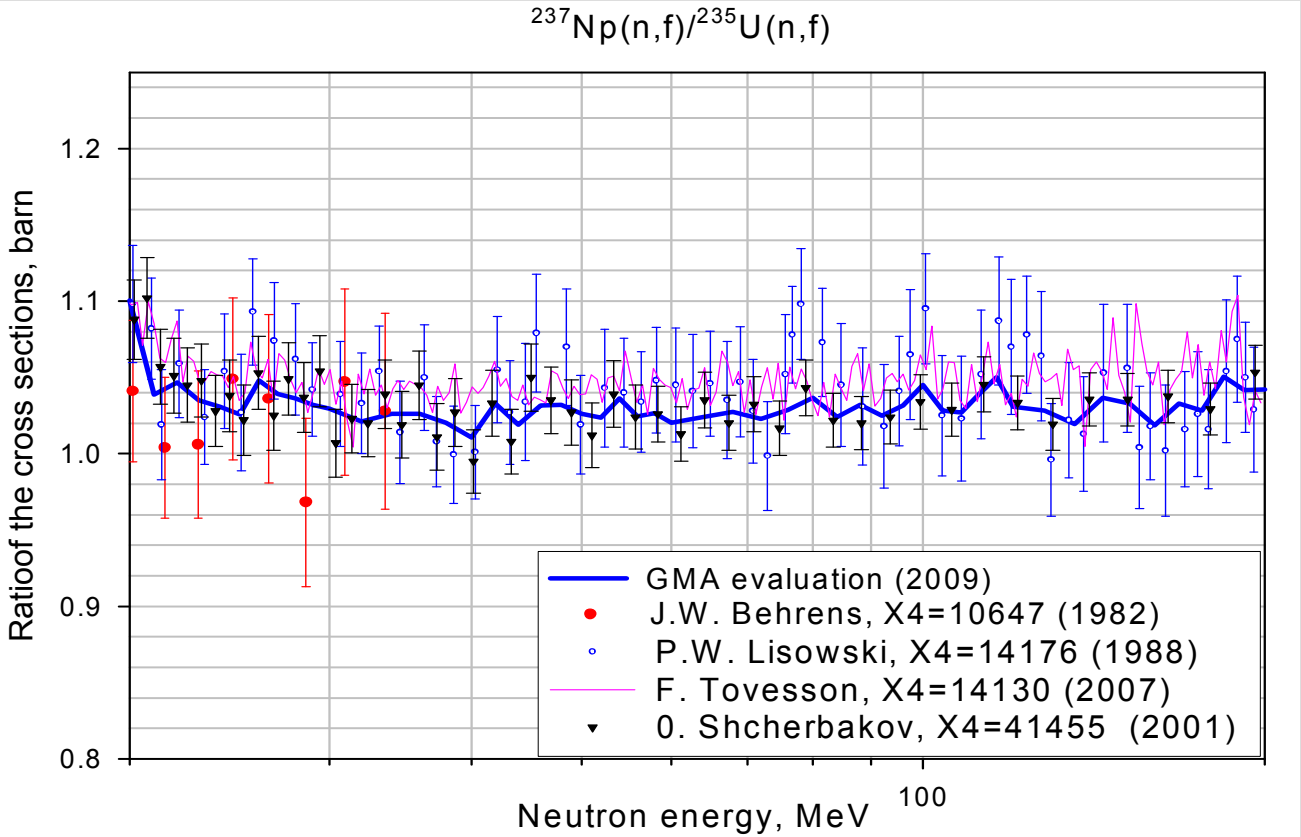
^{237}Np capture cross section, obtained in the combined evaluation with the standards.

GMA code and sim ultaneous evaluat ion of standards and minor actinides



^{237}Np fission cross section, obtained in the combined evaluation with the standards.

GMA code and sim ultaneous evaluat ion of standards and minor actinides



^{237}Np/^{235}U ratio of fission cross section, obtained in the combined evaluation with the standards in the energy range 20 – 200 MeV.

GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission

• GMA method allows also to make simultaneous evaluation of the prompt fission neutron spectra (PFNS) for thermal neutron induced fission ^{235}U, ^{239}Pu and ^{233}U combined with PFNS from spontaneous fission of ^{252}Cf (taken as standard, W. Mannhart).

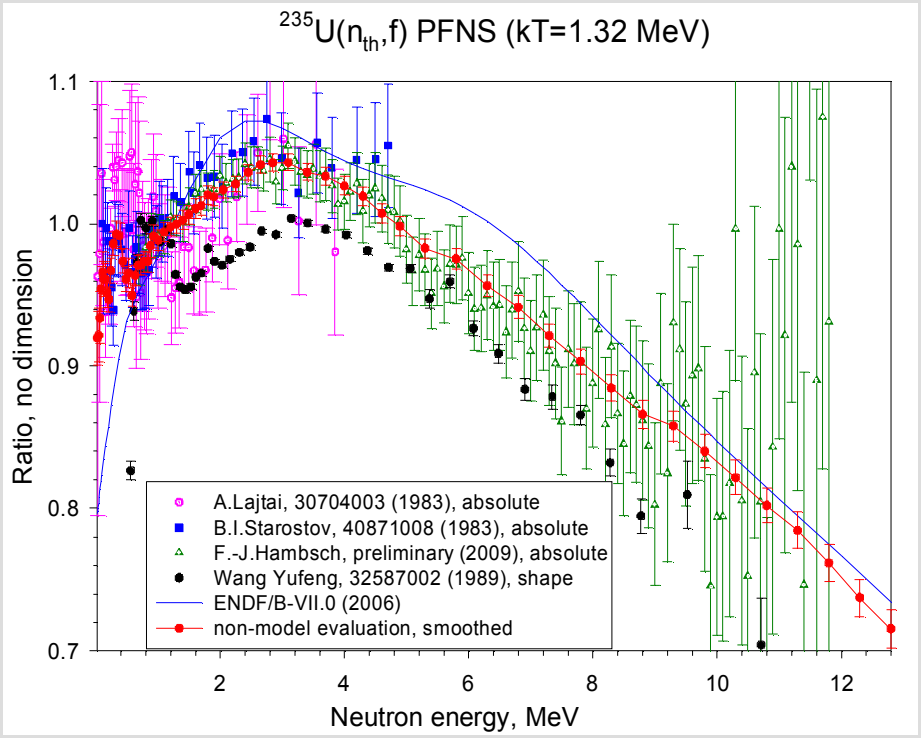
• Combined simultaneous evaluation of PFNS was done in the fission neutron energy range from 0.02 to 12.8 MeV, where are experimental data,

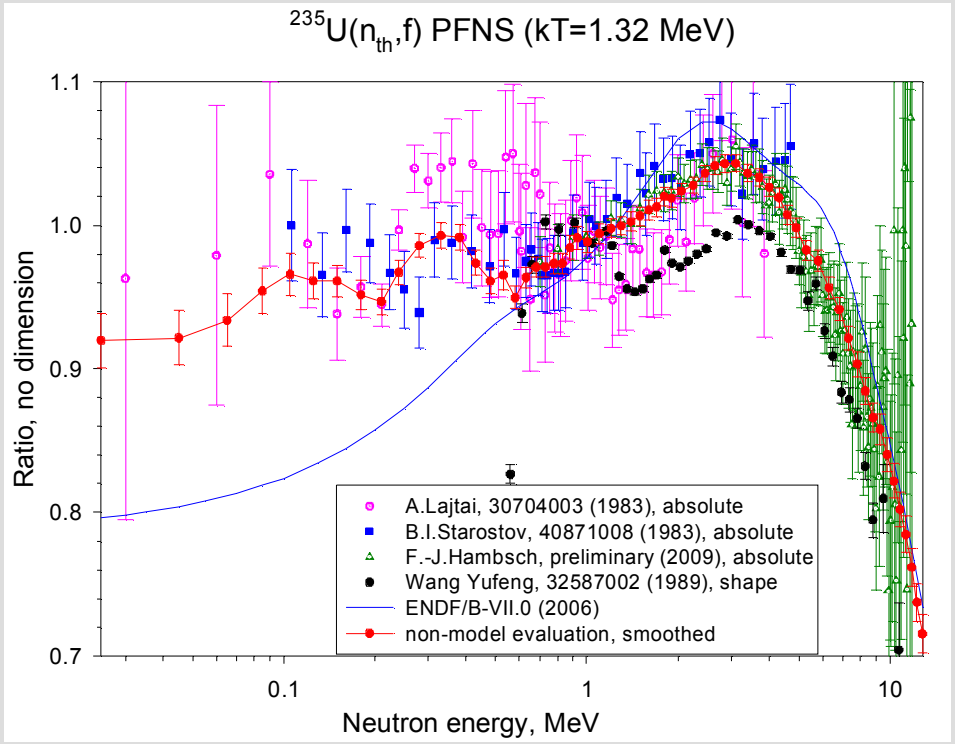
• In evaluation, all spectra (experimental and evaluated) were presented as the ratios to the Maxwellian spectrum with kT=1.32 MeV (to reduce the range of data variation).

• For energy range 0.02 to 12.8 МэВ, the requirements of the normalization of all spectra in this energy interval at the value 0.9985±0.0003 was set (constrain)

• Narrow energy range smoothing (covering 3 - 5 energy points) was used to avoid on of spectra due to normalization

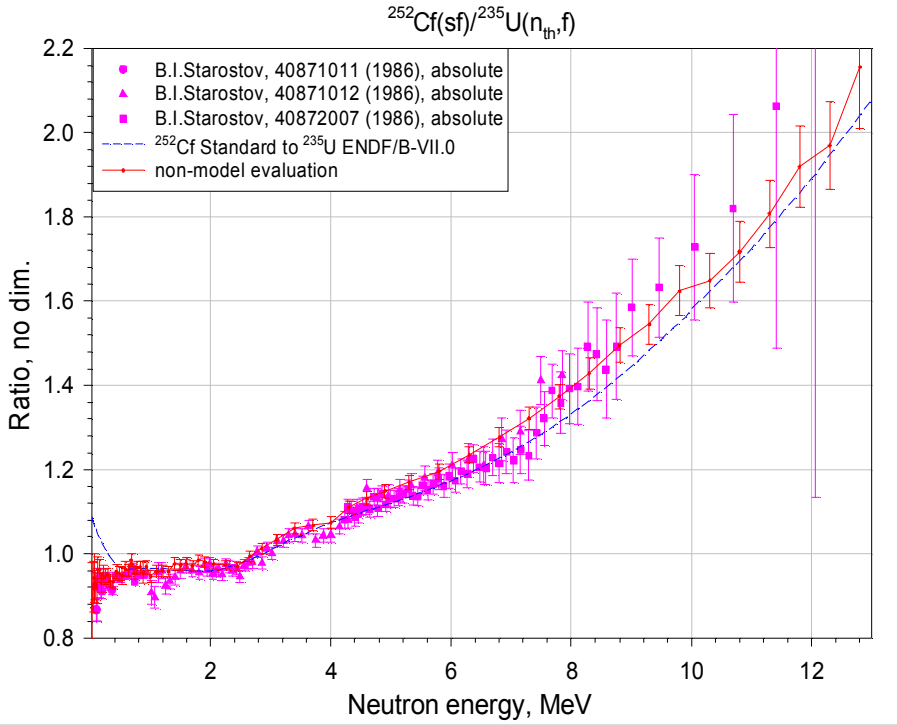
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results

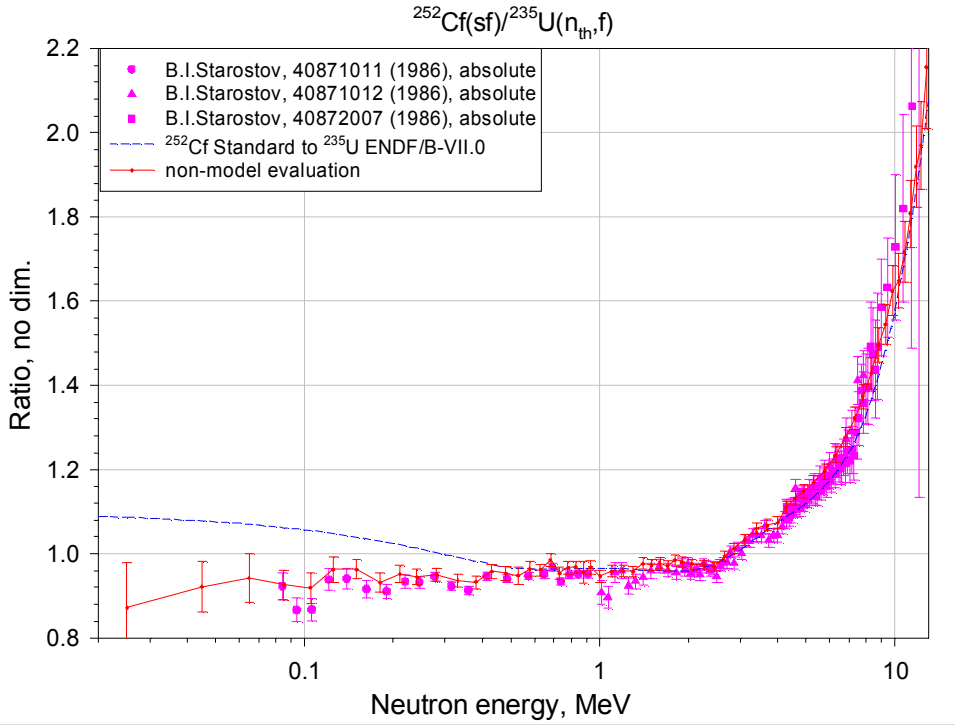




Comparison of the evaluated and experimental data on PFNS for $^{235}U(n_{th},f)$ in the linear and logarithmic scale the neutron energy. The results of absolute measurements and the measurements of the shape are shown.

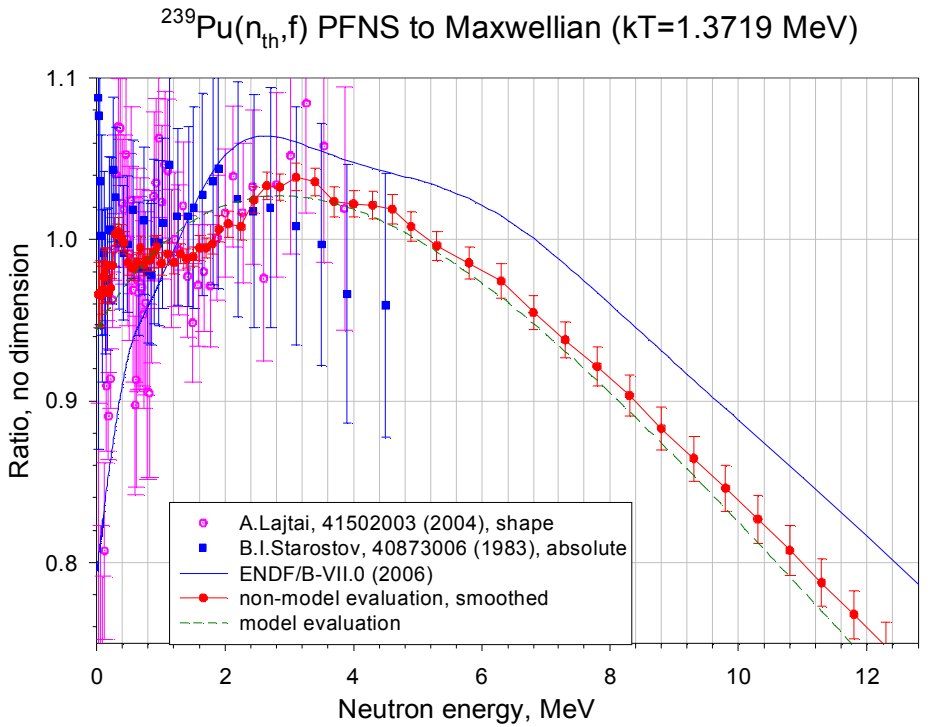
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results

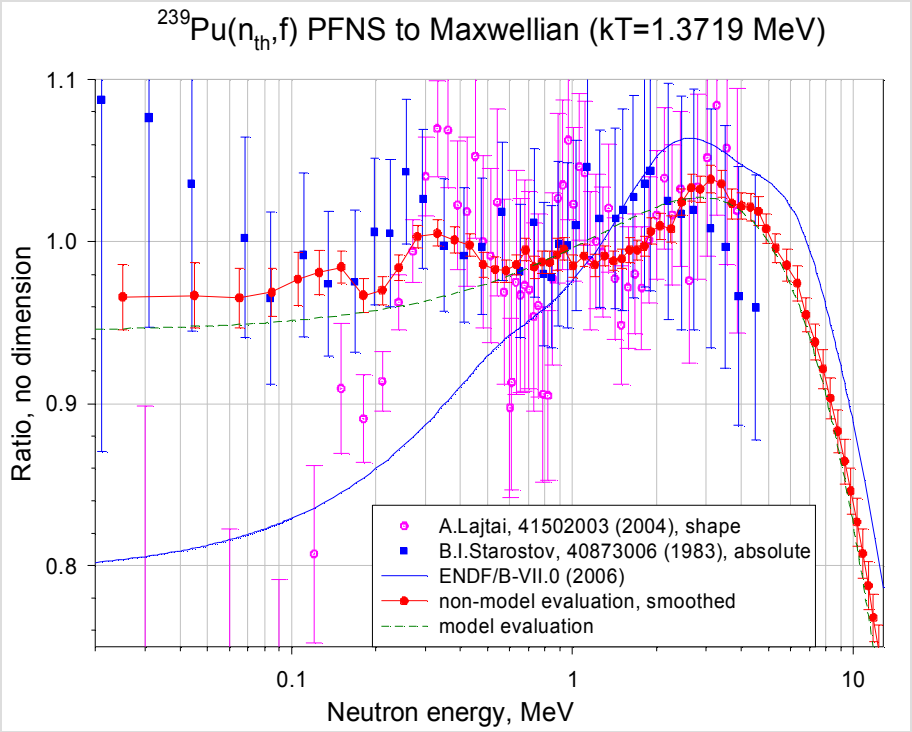




Comparison of the results of measurements of absolute ratio of the PFNS spectra ^{252}Cf(sf)/^{235}U(n$_{th}$,f) in linear and logarithmic scales on neutron energy.

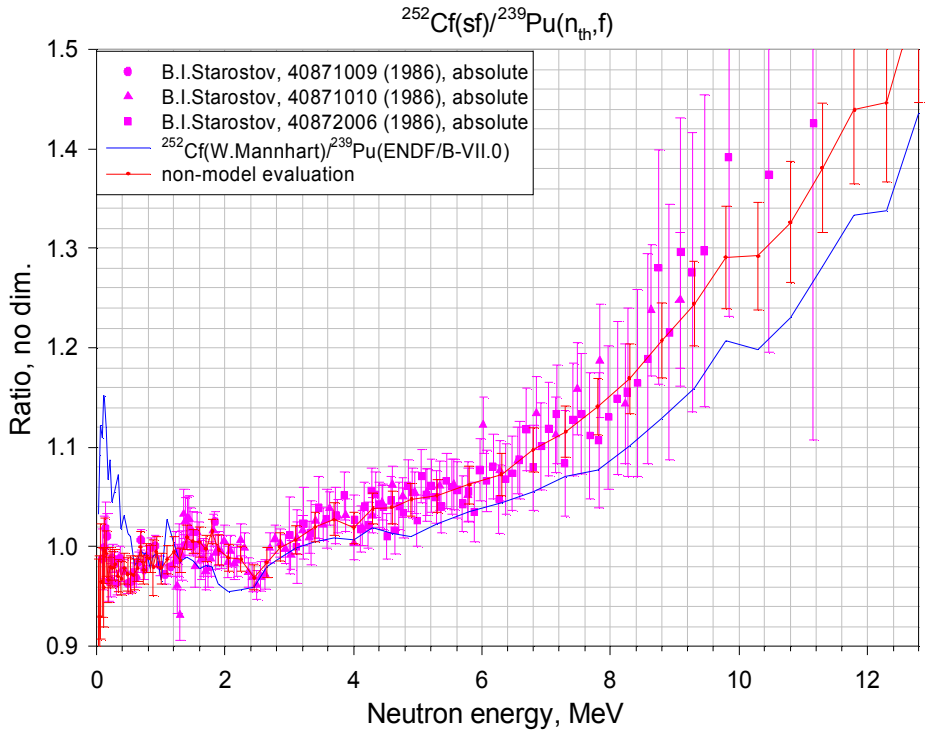
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results

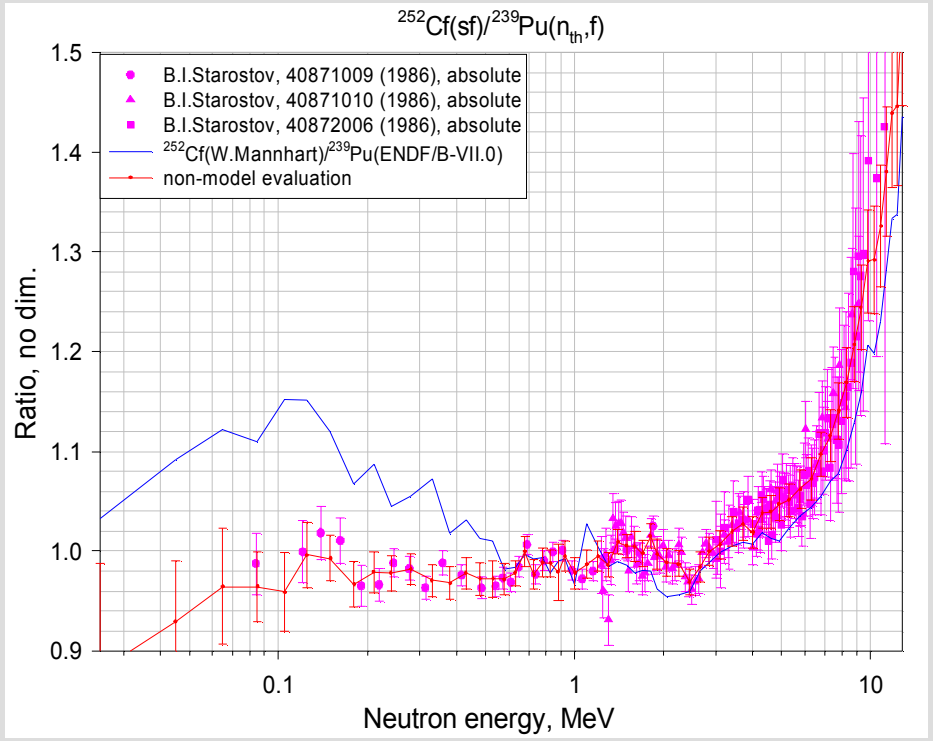




Comparison of the spectra of PFNS for ^{239}Pu(n$_{th}$,f) in linear or logarithmic scale on the neutron energy. The results of absolute and shape spectra measurements are shown.

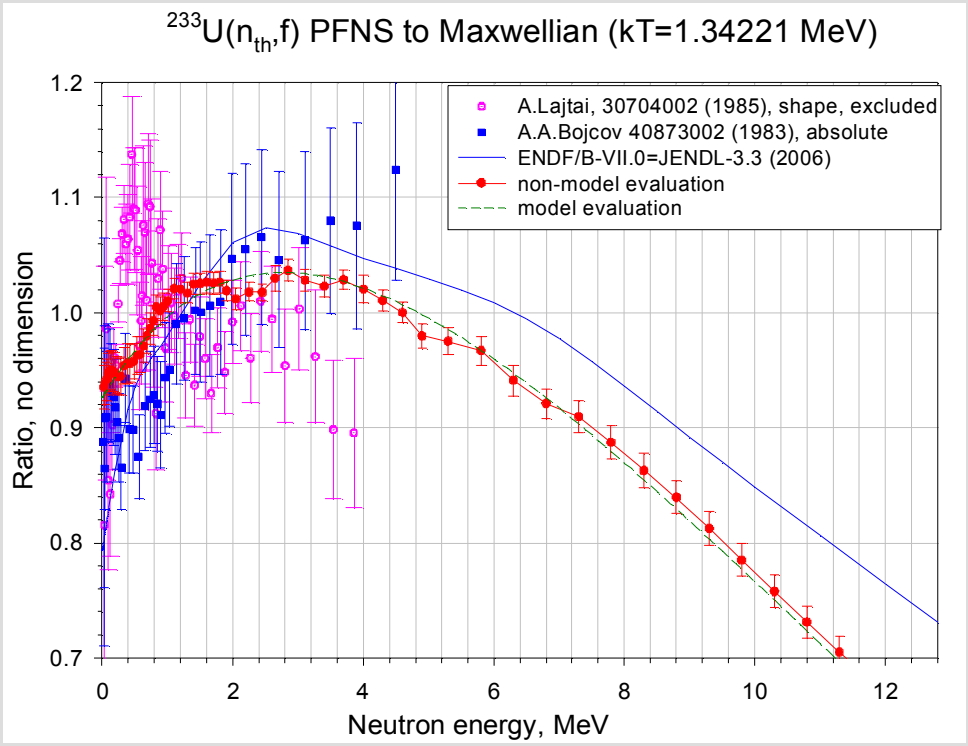
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results

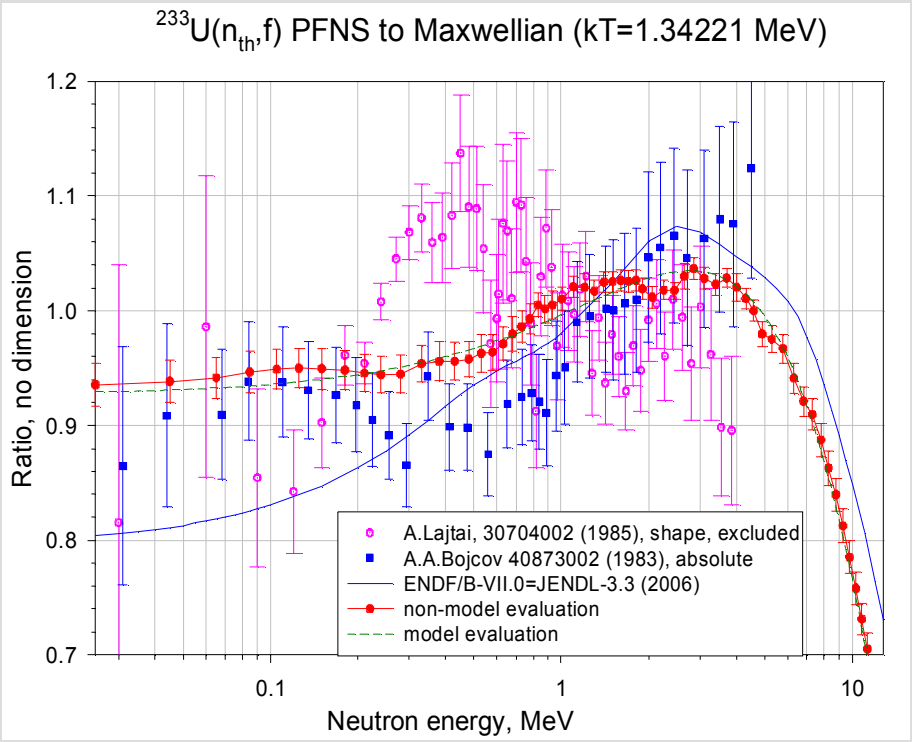




Comparison of the results of measurements of absolute ratio of the PFNS spectra ^{252}Cf(sf)/^{239}Pu(n$_{th}$,f) in linear and logarithmic scales on neutron energy.

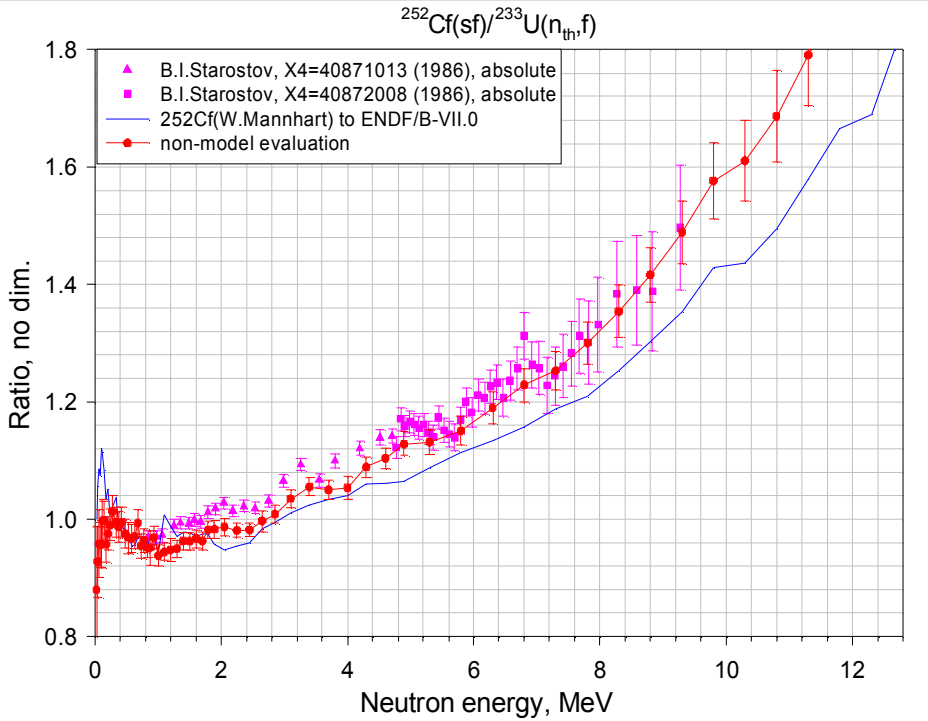
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results

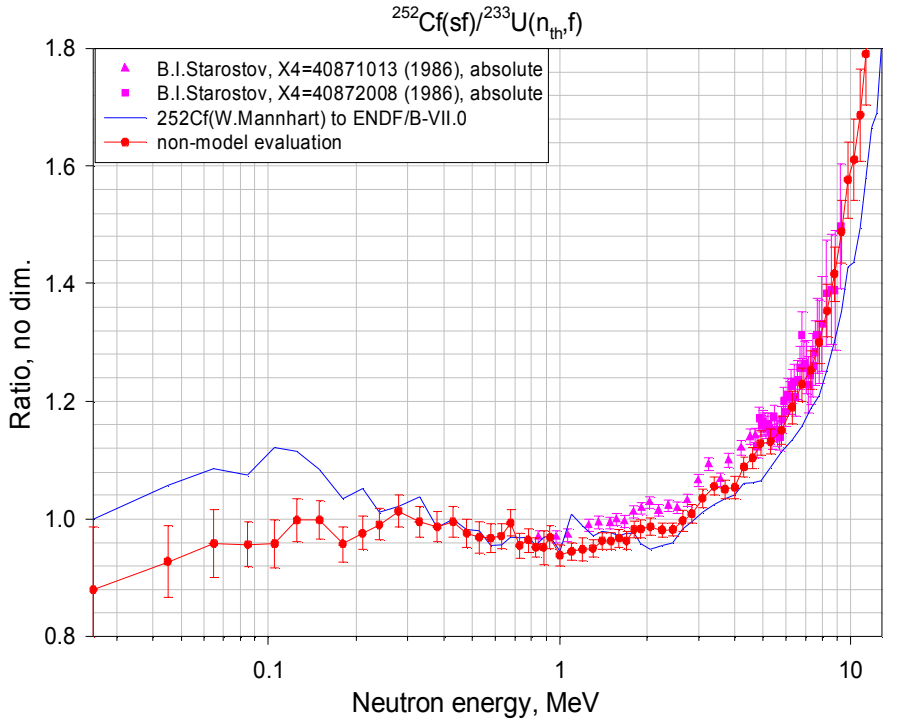




Comparison of the evaluated and experimental data on PFNS for ^{233}U(n$_{th}$,f) in the linear and logarithmic scale the neutron energy. The results of absolute measurements and the measurements of the shape are shown.

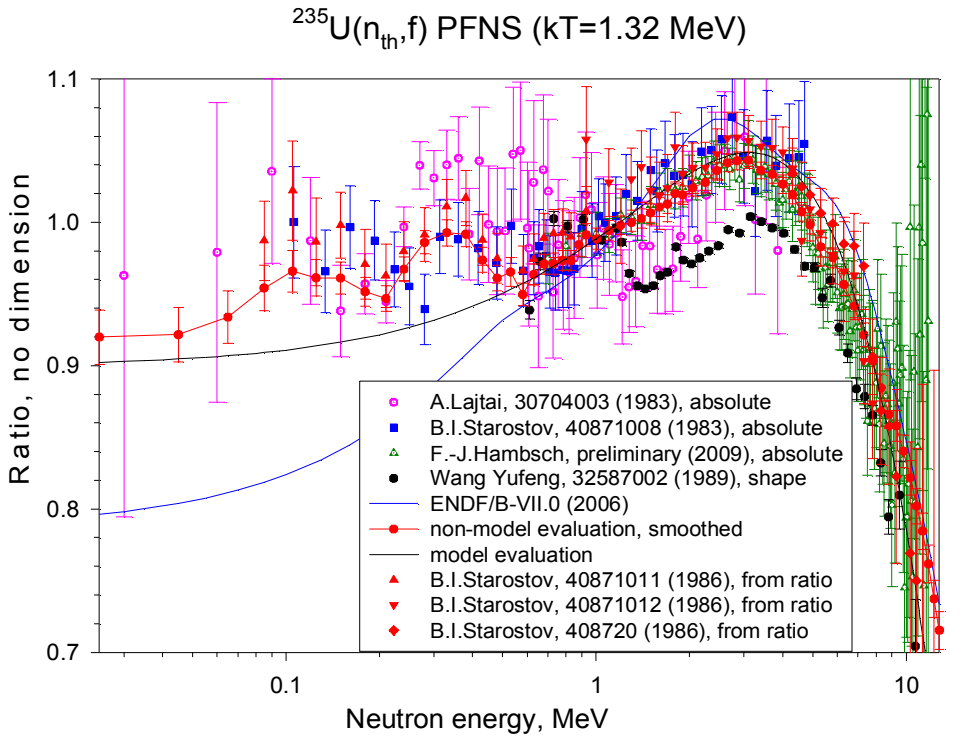
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results

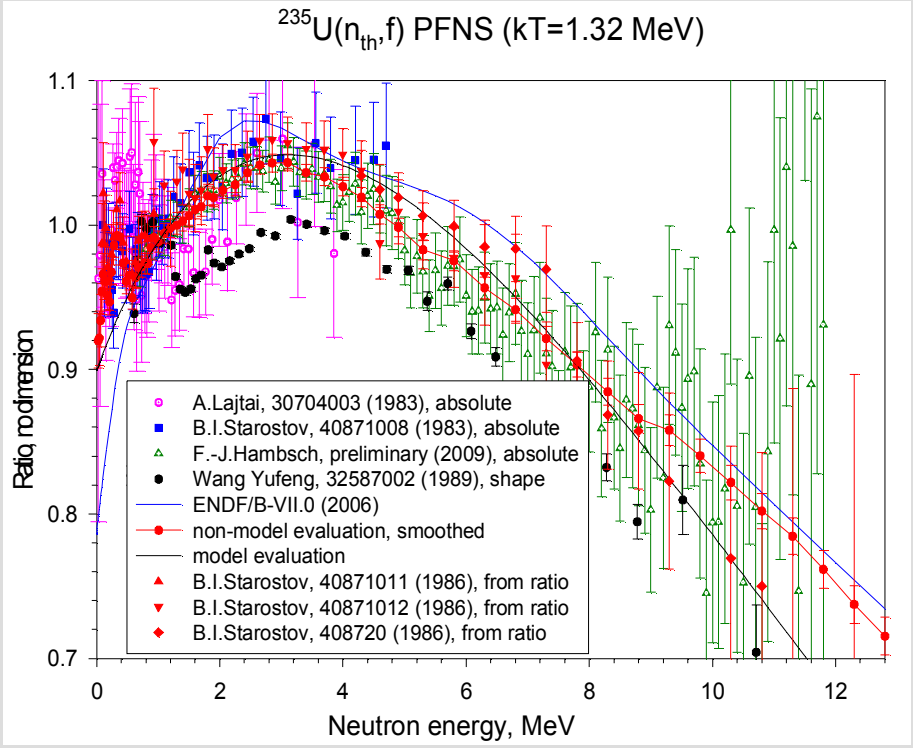




Comparison of the results of measurements of absolute ratio of the PFNS spectra ^{252}Cf(sf)/^{233}U(n$_{th}$,f) in linear and logarithmic scales on neutron energy.

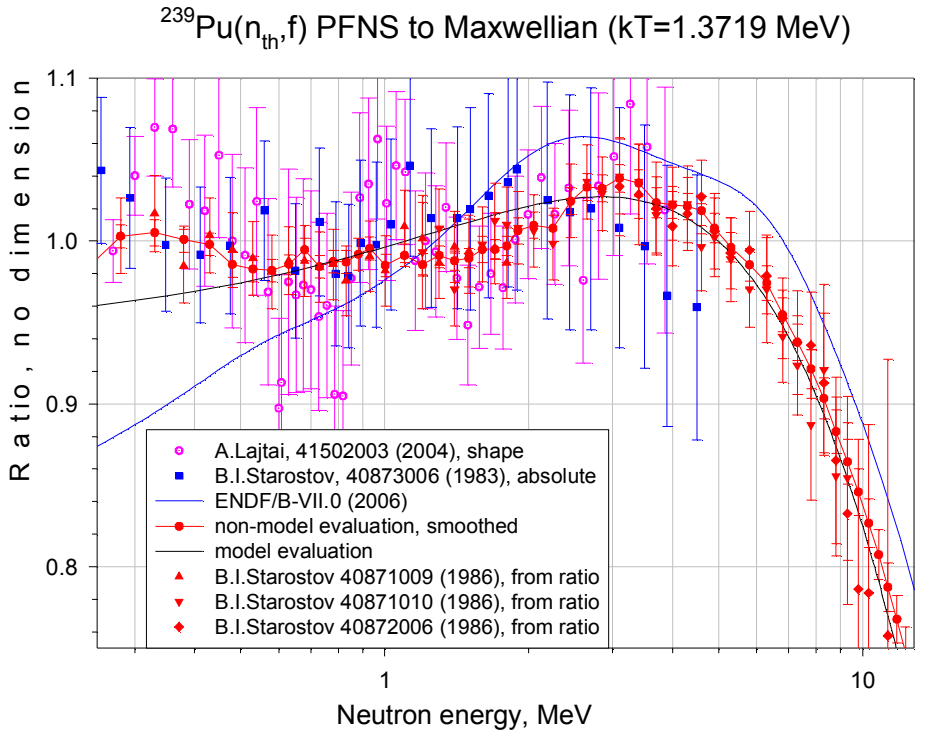
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results

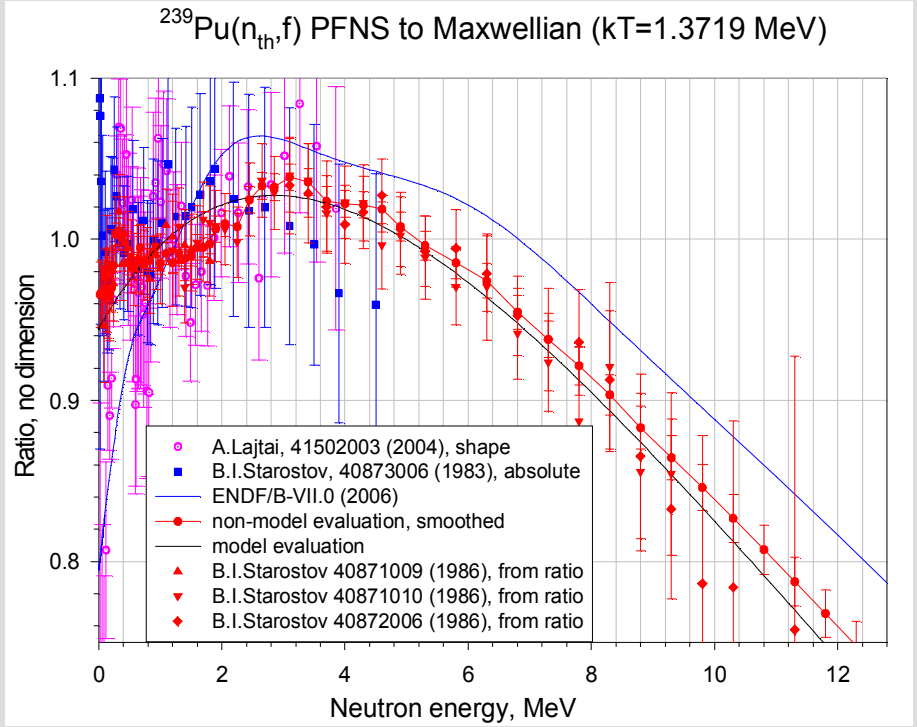




Comparison of the $^{235}U(n_{th},f)$ PFNS in linear and logarithmic scale on the neutron energy. Starostov's (NIIAR) data of absolute measurements of ratios were reduced to absolute spectra using new ^{252}Cf simultaneous evaluation. Results of the non-model and model evaluations are shown.

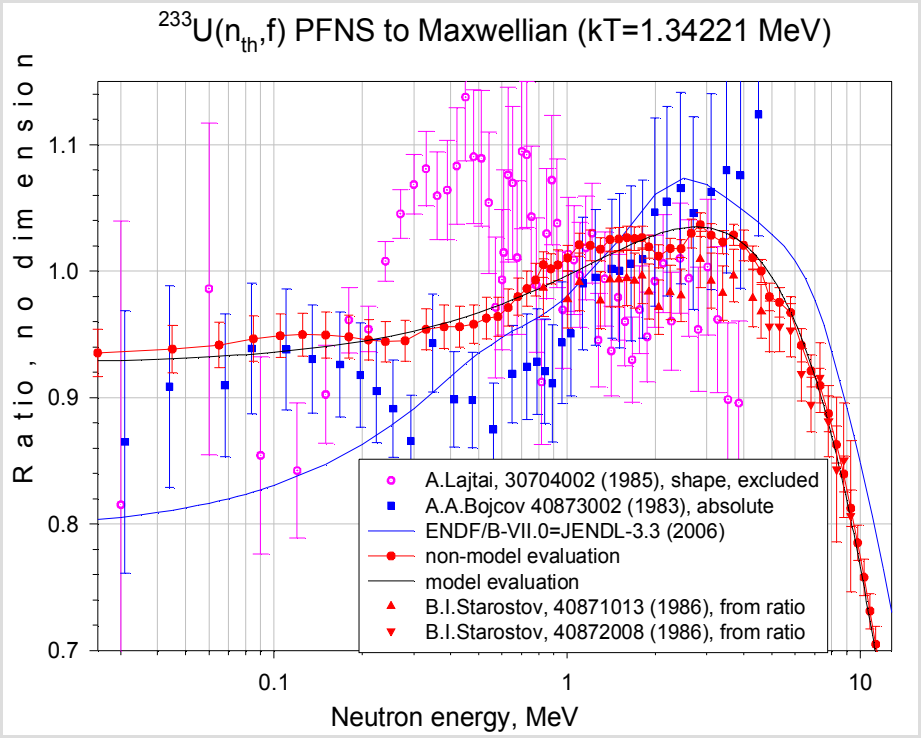
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results

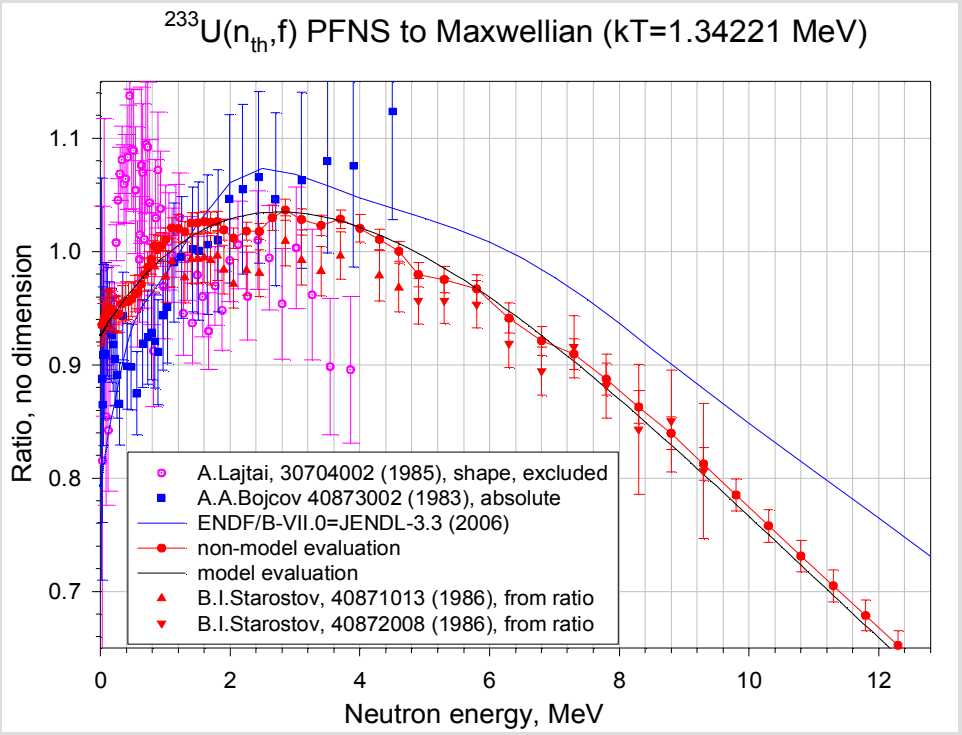




Comparison of the $^{239}Pu(n_{th},f)$ PFNS in linear and logarithmic scale on the neutron energy. Starostov (NIIAR) data of absolute measurements of ratios were reduced to absolute spectra using new ^{252}Cf simultaneous evaluation. Results of the non-model and model evaluations are shown.

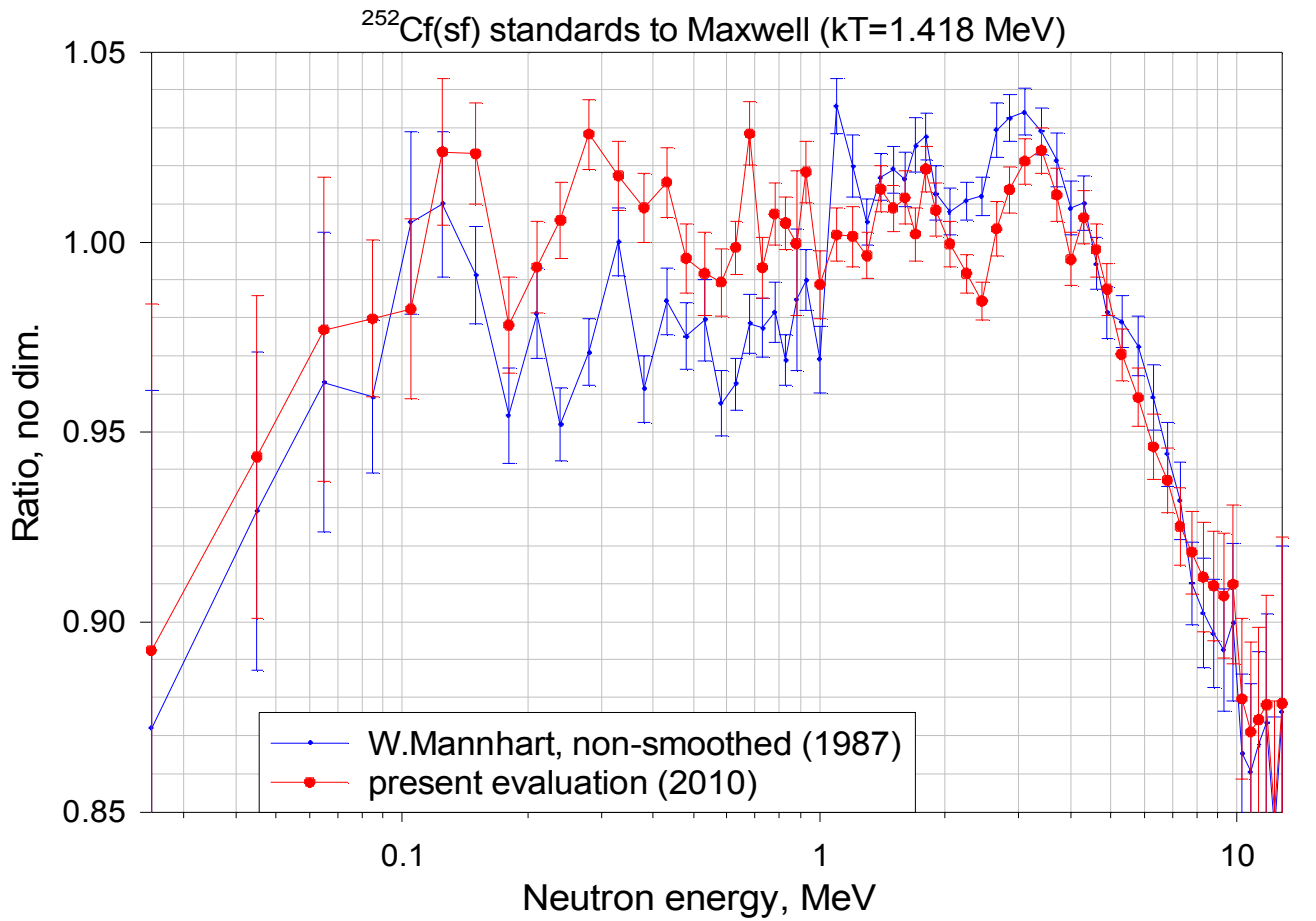
GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results





Comparison of the ^{233}U(n$_{th}$,f) PFNS in linear and logarithmic scale on the neutron energy. Starostov (NIIAR) data of absolute measurements of ratios were reduced to absolute spectra using new ^{252}Cf simultaneous evaluation. Results of the non-model and model evaluations are shown.

GMA code and simultaneous evaluation of prompt fission neutron spectra (PFNS) in thermal neutron induced fission: results



Comparison of new (combined) and old (based only at Cf spectrum measurements) evaluations of PFNS for ^{252}Cf(sf). Difference between red and blue evaluations shows the influence at ^{252}Cf(sf) spectrum evaluation from spectra of ^{235}U(n_{th},f), ^{233}U(n_{th},f) and ^{239}Pu(n_{th},f) in the combined fit of all data.

Lecture 2

Covariance matrix of uncertainties obtained in non-model and model fits of the sam e experimental data and Peelle's effect

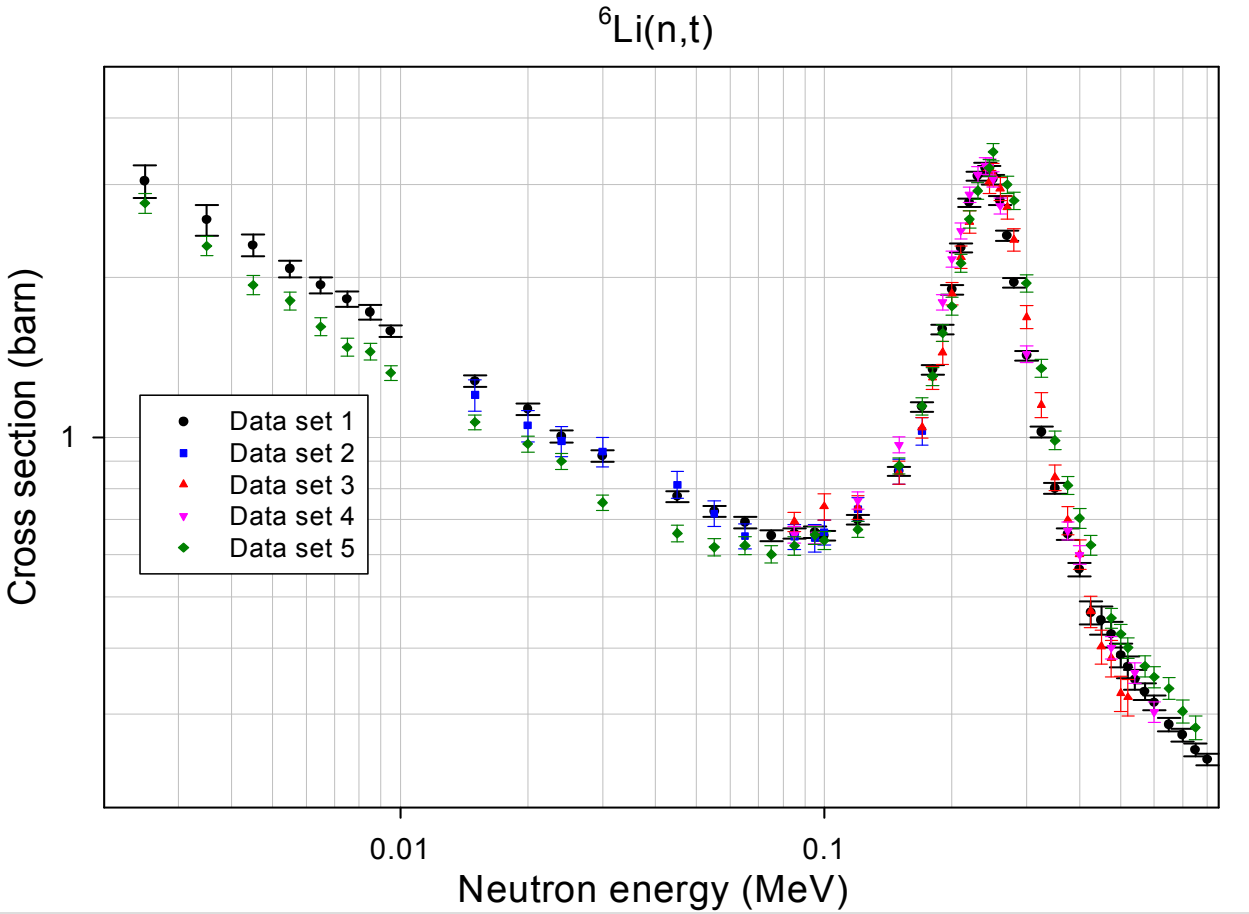
Model fits:

- number of parameters is less than number of data points,
- problems in the fit where chi-square multi-dimension parameter surface is complex
- matrix of sensitivity of the cross sections relative parameters is not unit matrix
- the evaluated data and covariances can be calculated in any energy nodes
- there is no ideal (absolutely true) models (e.g., “all world believe“ conception)

Non-model fits:

- number of parameters is equal to the number of the energy nodes in which data and covariances are evaluated
- fit is simple and straightforward
- matrix of sensitivity of the cross sections relative parameters is unit matrix
- evaluated data and covariances can be transformed only to wider energy bins

Covariance matrix of uncertainties obtained in non-model and model fits of the sam e experimental data and Peelle's effect

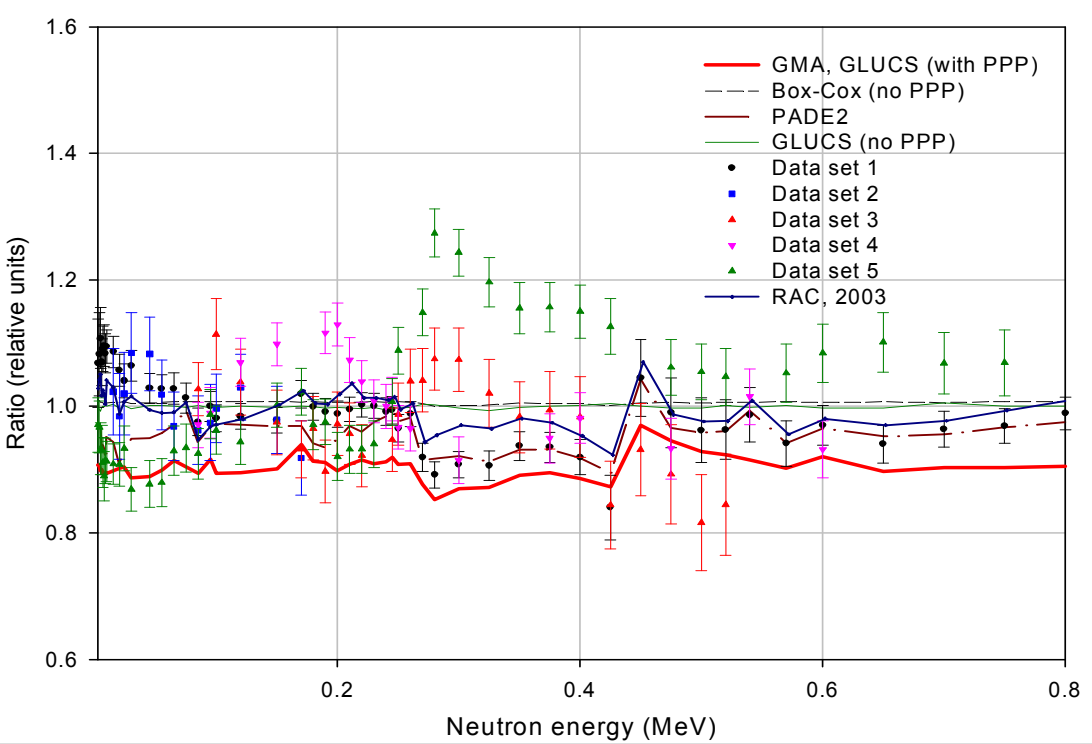


5 experimental data sets for ^{6}Li(n,t) reaction were selected for different test in the least-squares fit using model and non-model approaches.

data were rather discrepant and had large LERC components of the uncertainties

51 nodes on energy given in the range from 2.5 keV to 800 keV

Covariance matrix of uncertainties obtained in non-model and model fits of the same experimental data and Peelle's Pertinent Puzzle (PPP) effect

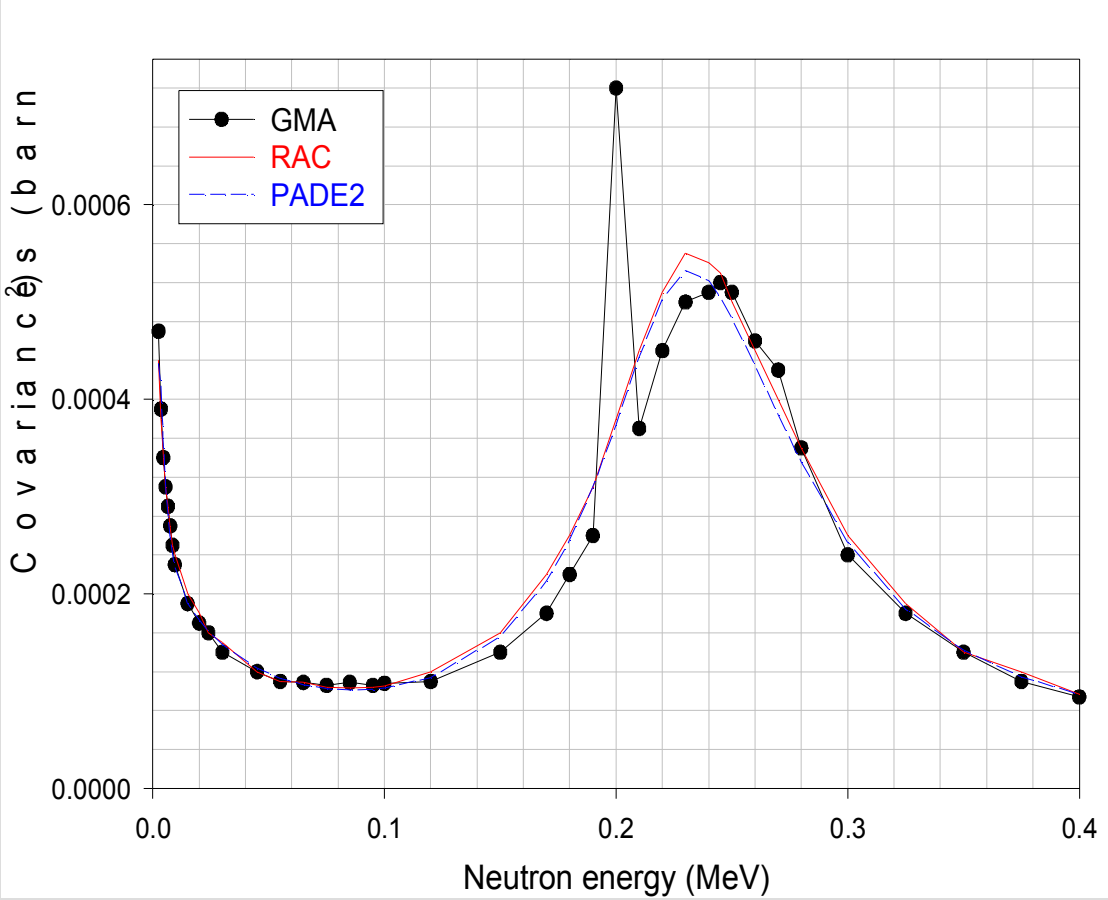


Results of the fit shown as ratio to GLUCS fit where PPP was excluded by technical fix (will be discussed later):

- non-model GMA and GLUCS without PPP exclusion
- polynomial model fit with Box-Cox transformation excluding PPP
- PADE2 analytical expansion model
- RAC R-matrix model fit

PPP effect is a visible bias of the evaluation relative the bulk of the experimental data in the least-squares fit caused by the ill-determined covariances of the experimental data

Covariance matrix of uncertainties obtained in non-model and model fits of the same experimental data and Peelle's Pertinent Puzzle (PPP) effect



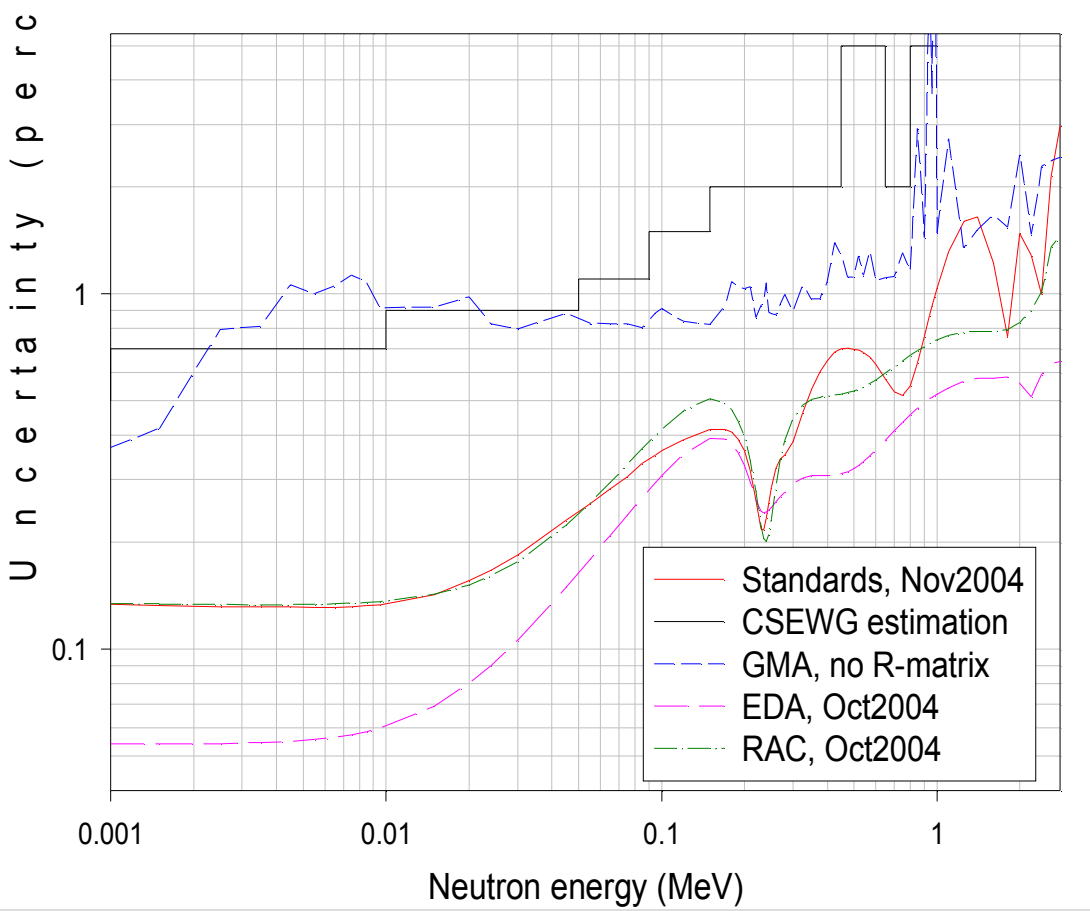
The row (column) of covariance matrix of uncertainties, which includes the variance for point at 0.2 MeV:

model fit reduces substantially the variances but increases the covariances near the diagonal

the sum of all elements for selected row (column) of covariance matrix practically does not depend from the type of the fit used (model or non-model)

PADE2 and RAC R-matrix are close models (pole expansions)

Covariance matrix of uncertainties obtained in non-model and model fits of the same experimental data and Peelle's Pertinent Puzzle (PPP) effect



- Per-cent uncertainties obtained in the fit of all available experimental data for ^{6}Li(n,t) reaction.
- EDA and RAC – two R-matrix codes wit different conceptions of accounting of uncertainties of experimental data
- EDA - only statistical uncertainties with free normalization of data
- RAC - full covariance matrix of experimental data is accounted
- CSEWG – expert estimation
- GMA – non-model it with all experimental data for ^{6}Li+n reactions

Peelle's (PPP) effect a nd m inimization o f i ts i nfluence a t the bias of the evaluation

PPP leads to the bias of the evaluation

The reason of the PPP lays in construction of the «unrealistic» covariance matrices of the uncertainties of the experimental data in cases of limited information about the components of the uncertainties of the data and their correlative properties

Taking two variables, S. Chiba and D. Smith had shown that if V_{11} and V_{22} are the diagonal elements of the covariance matrix of the uncertainties of the experimental data, V_{12} is an off-diagonal element and $V_{11} < V_{22}$, then in case of $|V_{12}| < V_{11}$ the PPP is absent

The practice had shown that the same is true in case of multivariate function, when $|V_{ij}| < V_{ii}$, for $V_{ii} < V_{jj}$), but this requires the proof

The PPP is fully absent, if the uncertainties of the experimental data have pure statistical nature and the covariance matrices of the relative uncertainties are used in the fit, or absolute covariance matrices obtained as a product of the relative covariance matrices of uncertainties at «true» value (or posterior evaluation) are used in the least-squares fit

Peelle's (PPP) effect and minimization of its influence at the bias of the evaluation

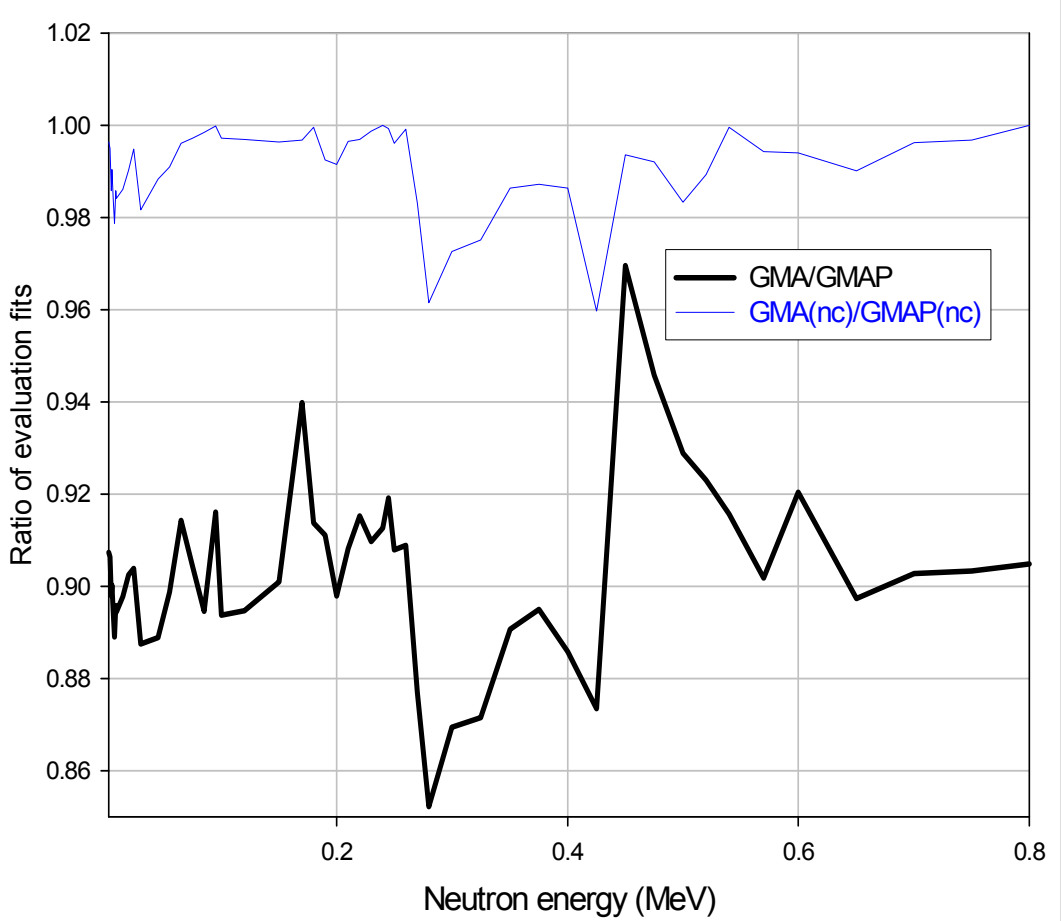
Because the posterior evaluation up to the moment of the finishing of the evaluation is not known, then, the iteration procedure can be used.

At the first step the prior evaluation is used instead of posterior and then the least-squares fit is repeated few times with the replacement at each step the old posterior evaluation at the new one up to the convergence.

In most cases only two - three iterations are needed before the prior and posterior evaluations are practically coincided.

This technical method of the PPP exclusion was proposed by S. Chiba and A. Smith and implemented in the GMA and GLUCS codes

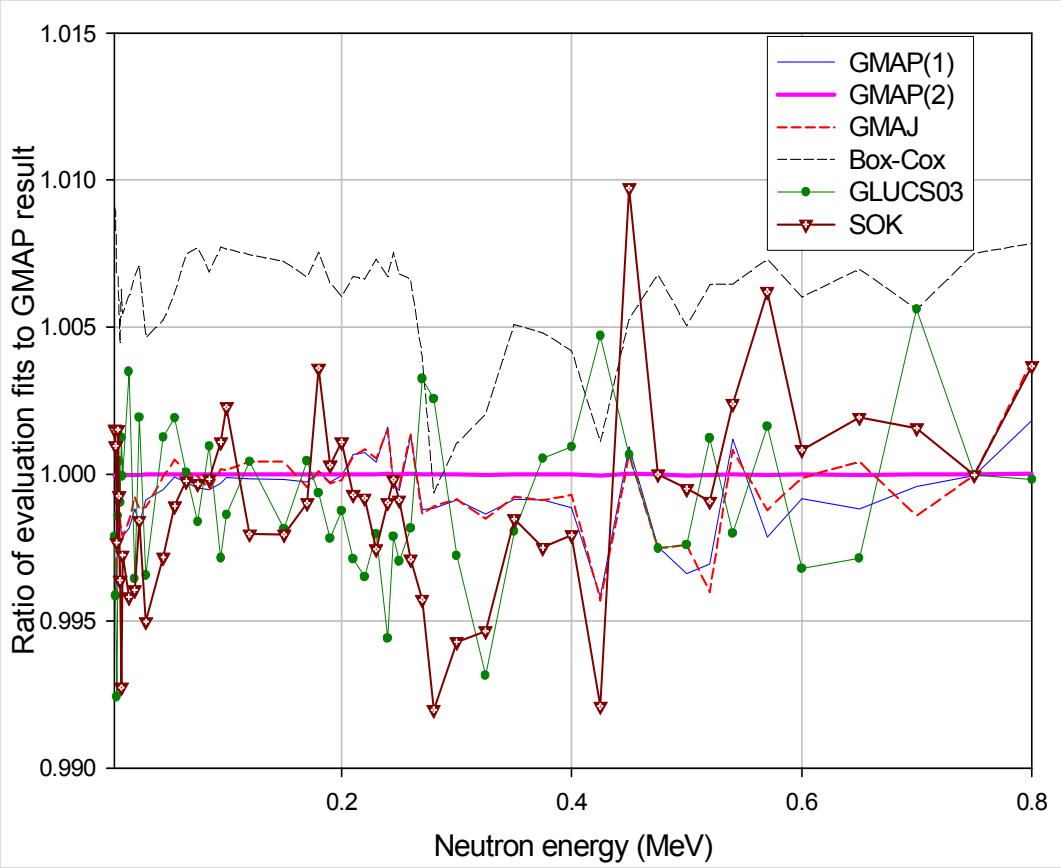
Peelle's (PPP) effect a nd m inimization o f i ts i nfluence a t the bias of the evaluation



PPP effects contains two components leading to the bias of the evaluation:

- mini-PPP (GMA(nc)/GMAP(nc) – even if no correlations, more lower data with the same % uncertainties as higher data are going in the fit with larger weight – see blue thin curve
- contribution of both effects of maxi-PPP and mini-PPP is shown by thick black curve – to exclude PPP, uncertainty of data with correlations are taken as relative uncertainties multiplied at posterior evaluated value

Peelle's (PPP) effect a nd m inimization o f i ts i nfluence a t the bias of the evaluation



Different technical fixes to avoid PPP:

- GMAP(1) and GMAP(2) — Chiba-Smith method for 1 and 2 iterations;
- GMAJ — GMA code rewritten by S. Chiba with 1 iteration;
- Box-Cox — use of Box-Cox transformation;
- GLUCS03 – GLUCS version with Chiba-Smith method;
- SOK – use of logarithm data transformations

Spread in the fit with different technical fixes of the PPP is in the limits of 0.3 – 0.5 %

Peelle's (PPP) effect and minimization of its influence at the bias of the evaluation

It was shown by Nancy Larson, that the “true”, unbiased evaluation can be obtained only if use the explicit method of construction of the covariance matrix of the uncertainties of the experimental data — method of propagation of the uncertainties starting from the primarily-measured quantities, *which all have only statistical type of uncertainties*.

For this, the model of the reduction of the primarily measured quantities, which depends from the method of the measurements, used detectors and introduced corrections should be explicitly given together with the statistical uncertainty of each parameter of the data reduction model

To large extent, this approach was implemented by Nancy Larson and co-workers in the code SAMMY, based on Bayesian search of the resonance parameters and fit of the cross sections in the resolved resonance region.

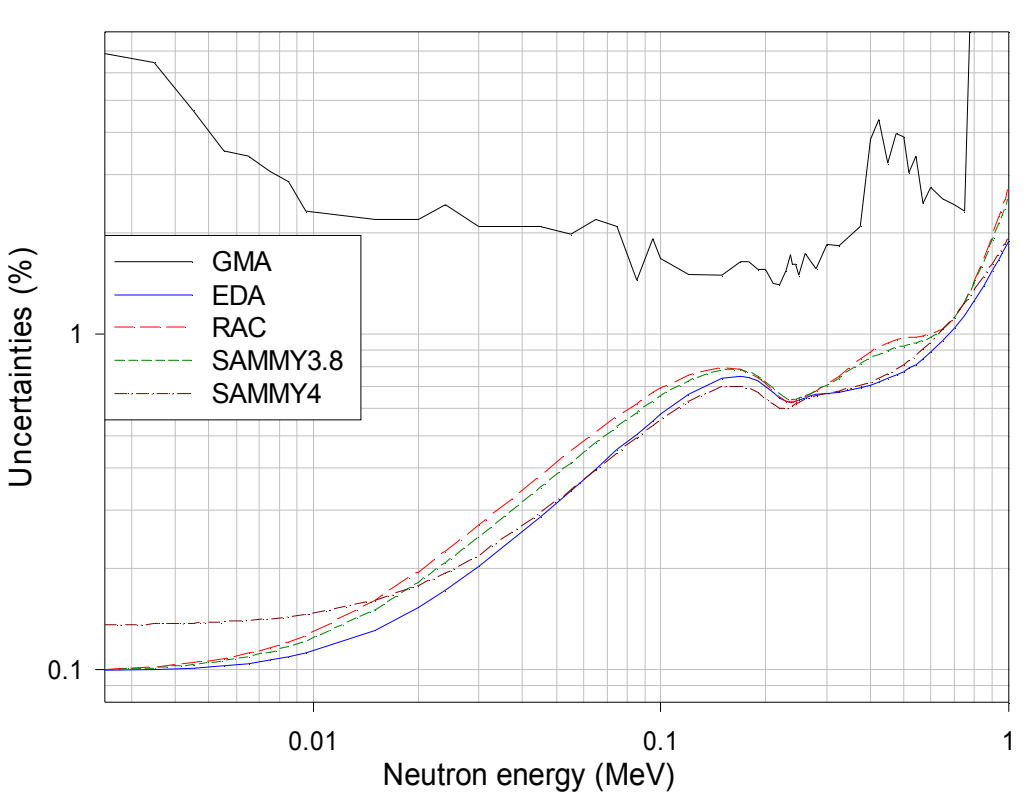
Effect of small uncertainties of the evaluated data. Reasons leading to small uncertainties

Uncertainties of the evaluated data are often compared on the per-cent error (uncertainty) of the data.

This is very incomplete and even often misleading comparison, because the full uncertainty of the evaluated data is characterized by the covariance matrix, where only the diagonal values have relations to the per-cent uncertainties.

Uncertainties of the evaluated data, obtained with the R-matrix code EDA, which does not account the systematic uncertainties in the fit of the large number of the experimental data, can be very low. For example, the uncertainty of the integral scattering elastic cross section of neutrons at the hydrogen in the thermal point can be close to 0.01 %, what causes natural doubts in the justification of the method, which gives such small evaluated uncertainties.

Effect of sm all uncert ainties of the evalu ated d ata. Reasons leading to small uncertainties



Per-cent uncertainties of the evaluated data obtained in the non-model and model fits of the same experimental data sets for ^{6}Li(n,t) reaction cross section (test2):

- GMA and RAC - non-model and R-matrix model fit of experimental data with SERC and LERC components of uncertainties
- EDA – R-matrix model with only SERC component of uncertainties accounted and free normalization (due to this EDA is on definition free from the PPP)
- SAMMY3.8 – SAMMY with RAC options
- SAMMY4 – SAMMY with EDA option

Low uncertainty of thermal value and *1/v* model energy dependence determines the low uncertainty of r-matrix fits in keV energy range

Effect of sm all uncert ainties of the evalu ated d ata. Reasons leading to small uncertainties

The reasons, leading to the substantial reducing of the uncertainties of the evaluated data:

- can be neglecting by some uncertainties
- neglect of the correlations between the components of the uncertainties, which are common for few experimental data sets. This relates, as a rule, to the measurements done in the same laboratory, at the same installation, with the same method, detectors and samples. Generally it is enough even to use the same samples in the measurements in different laboratories with different methods but have large component of uncertainties correlated between two data sets. Account of such correlations, for example in the evaluation of such important standard as ^{235}U(n,f), has a consequence that the minimal per-cent uncertainties even with large account of experimental data sets (186 sets of data with ^{235}U(n,f)) is never below 0.5 %.

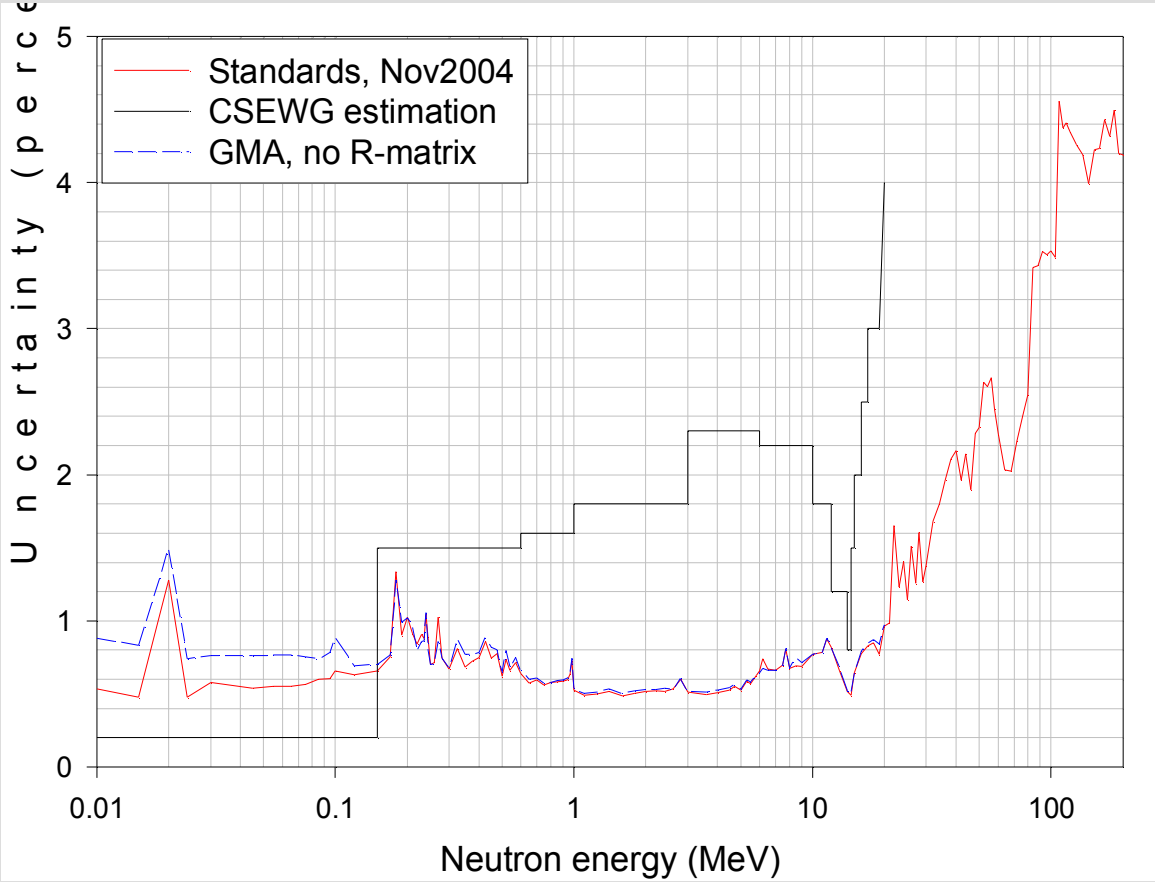
Effect of sm all uncert ainties of the evalu ated d ata. Reasons leading to small uncertainties

If in the fit of the data, the χ^2 per degree of freedom is larger than 1, important is the determination of the data sets, or range of the energies in these data sets, where are large discrepancies with other data (so-called «outliers»).

If it is impossible to understand and exclude the reason of these discrepancies, then uncertainty of these data should be increased. This will led to some increase of the uncertainties of the evaluated data.

The search of the outliers is rather difficult procedure, because for their identification, the knowledge of «true» values is needed. Because the true value “apriori” is not known, the iteration procedure should be organized with realistic prior evaluation at the first step. Thus, the iteration procedure with replacement of a prior evaluation at the next step by posterior evaluation is needed as for correction of the outlaying data, as well as for exclusion of the PPP effect.

Effect of sm all uncert ainties of the evalu ated d ata. Reasons leading to small uncertainties



Comparison of the per-cent uncertainties of the evaluated ^{235}U(n,f) neutron cross section standards with the expert's estimation (CSEWG) of the uncertainties which can be achieved in the modern experimental conditions (1987).

The reasons, why the uncertainty of the evaluated data in the energy range between 150 keV to 14 MeV are substantially lower than the expert estimation, is because in the evaluation 186 experimental data sets presenting 16 types of the data, which differ by the methods, detectors, types of used standards, including high-precision absolute measurements (based on associated particles method or hydrogen scattering standard) were used.

Effect of sm all uncert ainties of the evalu ated d ata. Reasons leading to small uncertainties

Experimental data can be measured with the use of different methods.

Each method of measurements may contain some systematical errors, corrections at which were not introduced or uncertainties related to them were not evaluated. We may consider them as hidden (or unrecognized) systematical uncertainties.

For revealing of these systematical uncertainties it is important to have a wide spectrum of measurements done with different methods or make new measurements which could be based at new method.

Evgeny Gai had developed the approach when in conditions of the sufficient number of the experimental data, additional (hidden) systematical component of the uncertainty in some energy interval for each data set was assigned using bias between the averaged data in this interval relative the arithmetical-averaged value for all data of this interval.

The use of this approach gives some information about possible non-accounted systematical uncertainty of each data set and increases the per-cent uncertainty in 1.5 — 2 times comparing with the approaches, where the conception of hidden systematical uncertainty of different methods had not been used.

Comparison of the covariance matrices of the uncertainties evaluated in the model and non-model fits and invariants of the uncertainties

As we seen, covariance matrices of the uncertainties of the evaluated data obtained in the model and non-model fits of the same experimental data are substantially different matrices. This causes serious problems in comparison of the uncertainties (it is impossible to compare large number of the matrix elements).

In many cases, in the comparison of the uncertainties, **only the diagonal elements of the matrices, or per-cent uncertainties** are taken into account. Such comparison is not complete and representative, and **can lead to the wrong conclusion about accuracy of the data**.

Comparison of the cov ariance m atrices of the uncertainties evaluated in the m odel and non-m odel fit s and invariants of the uncertainties

Practice of the evaluation allowed to fotmulate the following hypothesis for fits done at the same energy nodes:

«at model and non-model fits of the same sets of the experimental data by least-squares method, the sums of the elements of the covariance matrices of the uncertainties of the evaluated data obtained in these fits will be so close, up to what degree such fits are close»

Comparison of the covariance matrices of the uncertainties evaluated in the model and non-model fits and invariants of the uncertainties

Point #	Point #1		Point#25	
	GMA	RAC	GMA	RAC
1	0.00775	0.00158	0.00047	0.00044
2	0.00076	0.00123	0.00039	0.00038
3	0.00064	0.00102	0.00034	0.00034
4	0.00051	0.00086	0.00031	0.00031
5	0.00050	0.00076	0.00029	0.00029
6	0.00048	0.00067	0.00027	0.00027
7	0.00042	0.00060	0.00025	0.00025
8	0.00038	0.00055	0.00023	0.00024
20	0.00018	0.00019	0.00011	0.00012
21	0.00022	0.00024	0.00014	0.00016
22	0.00028	0.00029	0.00018	0.00022
23	0.00033	0.00032	0.00022	0.00026
24	0.00039	0.00038	0.00026	0.00031
25	0.00047	0.00044	0.00072	0.00038
26	0.00056	0.00053	0.00037	0.00045
27	0.00067	0.00064	0.00045	0.00051
28	0.00075	0.00074	0.00050	0.00055
29	0.00075	0.00080	0.00051	0.00054
30	0.00076	0.00082	0.00052	0.00053
47	0.000079	0.000076	0.000050	0.000052
48	0.000079	0.000068	0.000050	0.000050
49	0.000071	0.000064	0.000047	0.000048
50	0.000065	0.000064	0.000043	0.000045
51	0.000063	0.000067	0.000041	0.000041
Sum	0.023875	0.019656	0.011163	0.011191
Ratio of sums, model to Non-model	0.82		1.002	

Comparison of the covariances (in the units of barn^2) for 1-st and 25-th row (column) of the covariance matrices of the uncertainties for ^{6}Li(n,t) reaction evaluated at 51 nodes for 5 experimental data sets.

Large differences in the covariances at the diagonal or close to the diagonal. However, if we will sum up the elements of the matrices along the row (column), then the differences in the sums will be small, and total sums of all elements of covariance matrices differ at few per-cents.

Comparison of the cov ariance m atrices of the uncertainties evaluated in the m odel and non-m odel fit s and invariants of the uncertainties

The existence of such conserving quantity independent from the fit (***invariant***) could mean, that the uncertainties of many integral characteristics calculated with the data evaluated in different model and non-model fits will have non-substantial difference, although the covariance matrices of the uncertainties of these evaluations can look differently.

This invariant can be called as universal measure of the data uncertainties.

Comparison of the cov ariance m atrices of the uncertainties evaluated in the m odel and non-m odel fit s and invariants of the uncertainties

It is well known the invariant for covariance matrix of the spectrum (or any other function),
if constraint is set up,
that integral under evaluated spectrum (function) is precisely equal to the predetermined value (e.g., spectrum should be normalized at 1),
then the sum of all elements of covariance matrix should be equal to 0. In this case, the sum of all elements of covariance matrix along any row or column also should be equal 0.

Comparison of the covariance matrices of the uncertainties evaluated in the model and non-model fits and invariants of the uncertainties

Studies done by Evgeny Gai on the search of invariants of covariance matrices of the uncertainties revealed few forms with covariance matrices of the uncertainties, which are strict invariants.

If **R** is covariance matrix of uncertainties of experimental data,
G is matrix of the coefficients of the sensitivity,
T and -1 indexes mean transposing and inversion of the matrix,
then the least-squares method gives the covariance matrix of the evaluated parameters **W:**

$$\mathbf{W}=(\mathbf{G}^{T}\mathbf{R}^{-1}\mathbf{G})^{-1}$$

Covariance matrix **V** of the evaluated uncertainties in the nodes, where the experimental data are given can be written as: $\mathbf{V}=\mathbf{G}^{T}\mathbf{W}\mathbf{G}$

From here, spur (*Sp*) of the product of the matrices $\mathbf{R}^{-1}$ and **V** does not depend from the used model and quality of the fit determined by the χ^2 criterion and equals to the number of the model parameters *M* :

$$Sp\mathbf{R}^{-1}\mathbf{V}=\sum_{i,k}R^{-1}_{i,k}V_{k,i}=\sum_{i,k}\sum_{\alpha,\beta}R^{-1}_{i,k}G^{T}_{\alpha,i}W^{-1}_{\alpha,\beta}G_{\beta,k}=\sum_{\alpha,\beta}W_{\alpha,\beta}W^{-1}_{\alpha,\beta}=M$$

Comparison of the cov ariance m atrices of the uncertainties evaluated in the m odel and non-m odel fit s and invariants of the uncertainties

It can be shown also that, the following relations are strictly carried out for the models, which use the polynomial expansion, and only approximately for non-model fits by the least-squares method of the large number of the data sets:

$$\sum_{k,j} R^{-1}_{i,k} V_{k,j} = 1 \quad \text{for any line } i \text{ and:} \quad \sum_{i,k,j} R^{-1}_{i,k} V_{k,j} = N$$

$$Det(\mathbf{V} - \mathbf{R}) = 0,$$

where N is a number of data points (energy nodes) and *Det* is a determinant of the difference of two matrices given in the brackets. In the case of the polynomial models the quality of the fit does not influence at the strict equalities, but this is not so in the general case. All equalities are obtained analytically, basing at the conditions of the necessity and sufficiency of the solutions existing, and tested numerically using the PADE model of the analytical expansion. These relations can be used for the checking of the covariance matrices of the evaluated data obtained in different least-squares fits of the same experimental data.

Comparison of the covariance matrices of the uncertainties evaluated in the model and non-model fits and invariants of the uncertainties

It was also strictly shown for the evaluations with the model function of the regression type $y(x,p) = p_1 + g(x;p_2,...,p_M)$ with p_1 as a parameter of the constant shift, that the uncertainty of the weighted averaged value P_{wa} for evaluated data $y(x_k)$, where averaged values are determined as:

$$\bar{y}_{wa} = \frac{\sum_{i,k=1}^{N} R_{i.k}^{-1} y(x_k)}{\sum_{i,k=1}^{N} R_{i.k}^{-1}}$$

is a strict invariant, which does not depend from other characteristics of the model and depends only from the covariance matrix of uncertainties of the experimental data:

$$P_{wa} = <(\Delta\bar{y}_{wa})^2> = \frac{\sum R_{i,k}^{-1} V_{k,l} R_{l,m}^{-1}}{(\sum_{i,k} R_{i,k}^{-1})^2} = \frac{1}{(\sum_{i.k} R_{i,k}^{-1})}$$

Comparison of the cov ariance m atrices of the uncertainties evaluated in the m odel and non-m odel fit s and invariants of the uncertainties

Although the strict invariant for covariance matrix of the uncertainties of the evaluated data in case of any model was not found,

comparison of the sums of the elements of the covariance matrices of the uncertainties evaluated in different models,

or uncertainties of the integral quantities calculated with the evaluations obtained in different models,

gives more objective picture of the uncertainties comparison, then just comparison of their per-cent uncertainties.